2-Phenylethyl tiglate

Other names:	Phenylethyl tiglate 2-Butenoic acid, 2-methyl-, 2-phenylethyl ester, (E)- trans-2-Butenoic acid, 2-methyl-, phenethyl ester Phenethyl tiglate Phenylethyl «alpha»-methylbutenoate, (E)- «beta»-Phenylethyl tiglate 2-Phenylethyl (2E)-2-methyl-2-butenoate trans-2-Methyl-2-butenoic acid, phenethyl ester 2-Phenylethyl (E)-2-methyl-2-butenoate Phenylethyl (E)-2-methyl-2-butenoate 2-Butenoic acid, 2-methyl-, 2-phenylethyl ester, (2E)- 2-Phenylethanol tiglate phenethyl 2-methylcrotonate
Inchi:	InChI=1S/C13H16O2/c1-3-11(2)13(14)15-10-9-12-7-5-4-6-8-12/h3-8H,9-10H2,1-2H3/b11
InchiKey:	KVMWYGAYARXPOL-QDEBKDIKSA-N
Formula:	C13H16O2
SMILES:	CC=C(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	204.26
CAS:	55719-85-2

Physical Properties

Property code	Value	Unit	Source
gf	8.74	kJ/mol	Joback Method
hf	-212.49	kJ/mol	Joback Method
hfus	25.15	kJ/mol	Joback Method
hvap	56.00	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.738		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1584.00		NIST Webbook

rinpol	1590.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1598.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1589.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2226.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2214.00		NIST Webbook
ripol	2214.00		NIST Webbook
ripol	2227.00		NIST Webbook
ripol	2210.00		NIST Webbook
ripol	2188.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2227.00		NIST Webbook
tb	603.85	K	Joback Method
tc	818.90	K	Joback Method
tf	315.81	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.85	J/mol×K	603.85	Joback Method
cpg	438.37	J/mol×K	639.69	Joback Method
cpg	452.94	J/mol×K	675.53	Joback Method
cpg	466.59	J/mol×K	711.37	Joback Method
cpg	479.36	J/mol×K	747.21	Joback Method
cpg	491.29	J/mol×K	783.06	Joback Method

cpg	502.43	J/mol×K	818.90	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55719852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume