BENZYL TIGLATE

Other names: 2-Butenoic acid, 2-methyl-, phenylmethyl ester, (E)-
trans-2-Butenoic acid, 2-methyl-, phenylmethyl ester
benzyl 2-methylcrotonate
Inchi: InChI=1S/C12H14O2/c1-3-10(2)12(13)14-9-11-7-5-4-6-8-11/h3-8H,9H2,1-2H3/b10-3+
InchiKey: QRGSTISKDZCDHV-XCVCLJGOSA-N
Formula: C12H14O2
SMILES: C/C=C(\C)C(=O)OCc1ccccc1
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
hf	-230.96	kJ/mol	Cheméo Relay (1.0)
hfus	22.56	kJ/mol	Joback Method
hvap	67.27	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-3.34		Cheméo Relay (1.0)
logp	2.696		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
rinpol	1466.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1499.00		NIST Webbook
ripol	2103.00		NIST Webbook

ripol	2075.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2106.00		NIST Webbook
ripol	2104.00		NIST Webbook
ripol	2114.00		NIST Webbook
ripol	2110.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2147.00		NIST Webbook
tb	523.27	K	Cheméo Relay (1.0)
tf	246.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.15	J/mol×K	580.97	Joback Method
cpg	389.04	J/mol×K	617.44	Joback Method
cpg	402.99	J/mol×K	653.92	Joback Method
cpg	416.04	J/mol×K	690.39	Joback Method
cpg	428.24	J/mol×K	726.86	Joback Method
cpg	439.62	J/mol×K	763.34	Joback Method
cpg	450.23	J/mol×K	799.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37526888&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point