Phenylacetic acid, 3-methylbut-2-enyl ester

Inchi:	InChI=1S/C13H16O2/c1-11(2)8-9-15-13(14)10-12-6-4-3-5-7-12/h3-8H,9-10H2,1-2H3
InchiKey:	AJONNXSYRQWSAE-UHFFFAOYSA-N
Formula:	C13H16O2
SMILES:	CC(C)=CCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	204.26
CAS:	151091-17-7

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	1549.30		NIST Webbook
rinpol	1549.30		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

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=C151091177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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