Bornyl isobutyrate

Other names:	bornyl isobutanoate
	endo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl isobutyrate
Inchi:	InChI=1S/C14H24O2/c1-9(2)12(15)16-11-8-10-6-7-14(11,5)13(10,3)4/h9-11H,6-8H2,1-5
InchiKey:	KRKIAJBQOUBNSE-UHFFFAOYSA-N
Formula:	C14H24O2
SMILES:	CC(C)C(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	224.34
CAS:	50277-27-5

Physical Properties

Property code	Value	Unit	Source
gf	-86.36	kJ/mol	Joback Method
hf	-453.13	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	52.60	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.400		Crippen Method
mcvol	193.840	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1402.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1402.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1638.00		NIST Webbook
tb	604.46	K	Joback Method
tc	817.37	K	Joback Method
tf	376.38	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.35	J/mol×K	604.46	Joback Method
cpg	560.28	J/mol×K	639.94	Joback Method
cpg	579.13	J/mol×K	675.43	Joback Method
cpg	597.14	J/mol×K	710.91	Joback Method
cpg	614.49	J/mol×K	746.40	Joback Method
cpg	631.42	J/mol×K	781.88	Joback Method
cpg	648.14	J/mol×K	817.37	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C50277275&Units=SI

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

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