Bornyl propanoate

Other names: endo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl propionate
Bornyl propionate
Inchi: InChI=1S/C13H22O2/c1-5-11(14)15-10-8-9-6-7-13(10,4)12(9,2)3/h9-10H,5-8H2,1-4H3/t9
InchiKey: FAFMZORPAAGQFV-NRUUGDAUSA-N
Formula: C13H22O2
SMILES: CCC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 210.31
CAS: 78548-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-92.34	kJ/mol	Joback Method
hf	-427.21	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.154		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1362.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1641.00		NIST Webbook
tb	582.02	K	Joback Method
tc	794.09	K	Joback Method
tf	380.11	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.22	J/mol×K	582.02	Joback Method
cpg	507.29	J/mol×K	617.37	Joback Method
cpg	525.26	J/mol×K	652.71	Joback Method
cpg	542.34	J/mol×K	688.06	Joback Method

cpg	558.72	J/mol×K	723.40	Joback Method
cpg	574.62	J/mol×K	758.75	Joback Method
cpg	590.26	J/mol×K	794.09	Joback Method
hvapt	55.90	kJ/mol	422.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78548535&Units=SI
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

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
hvapt:	Enthalpy of vaporization at a given temperature
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