Isobornyl thiocyanoacetate

Other names:	Acetic acid, thiocyanato-, 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, exo-
	Acetic acid, thiocyanato-, isobornyl ester
	Acetic acid, thiocyanato-, isobornyl ester, exo-
	Bornate
	Cidalon
	Isobornyl thiocyanatoacetate
	Terpinyl thiocyanoacetate
	Thanisol
	Thanite
	ENT 92
	Isoborneol, thiocyanatoacetate
	Thiocyanatoacetic acid isobornyl ester
	Acetic acid, thiocyanato-, 1,7,7-trimethylbicyclo(2,2,1)hept-2-yl ester, exo-
	Isobornylester kyseliny thiokyanatooctove
	Acetic acid, 2-thiocyanato-, (1R,2R,4R)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, rel-
	Acetic acid, thiocyanato-, (1R,2R,4R)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, rel-
	NSC 3552
	1,7,7-trimethylbicyclo[2.2.1]hept-2-yl thiocyanatoacetate
Inchi:	InChI=1S/C13H19NO2S/c1-12(2)9-4-5-13(12,3)10(6-9)16-11(15)7-17-8-14/h9-10H,4-7H2
InchiKey:	IXEVGHXRXDBAOB-RUETXSTFSA-N
Formula:	C13H19NO2S
SMILES:	CC1(C)C2CCC1(C)C(OC(=O)CSC#N)C2
Mol. weight [g/mol]:	253.36
CAS:	115-31-1

Physical Properties

Property code	Value	Unit	Source
gf	73.96	kJ/mol	Joback Method
hf	-220.46	kJ/mol	Joback Method
hfus	21.57	kJ/mol	Joback Method
hvap	68.06	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.959		Crippen Method
mcvol	197.480	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1790.00		NIST Webbook
tb	752.88	K	Joback Method

tc	993.05	K	Joback Method
tf	479.50	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.17	J/mol×K	752.88	Joback Method
cpg	598.04	J/mol×K	792.91	Joback Method
cpg	614.78	J/mol×K	832.94	Joback Method
cpg	631.70	J/mol×K	872.97	Joback Method
cpg	649.08	J/mol×K	913.00	Joback Method
cpg	667.21	J/mol×K	953.03	Joback Method
cpg	686.38	J/mol×K	993.05	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=C115311&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