Borneol, trifluoroacetate (ester)

Other names: Borneol, trifluoroacetate
Inchi: InChI=1S/C12H17F3O2/c1-10(2)7-4-5-11(10,3)8(6-7)17-9(16)12(13,14)15/h7-8H,4-6H2,1
InchiKey: LINNXWGLYUPPJS-UHFFFAOYSA-N
Formula: C12H17F3O2
SMILES: CC1(C)C2CCC1(C)C(OC(=O)C(F)(F)F)C2
Mol. weight [g/mol]: 250.26
CAS: 28587-55-5

Physical Properties

Property code	Value	Unit	Source
gf	-682.35	kJ/mol	Joback Method
hf	-1003.65	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	44.79	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.307		Crippen Method
mcvol	170.970	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1129.00		NIST Webbook
tb	553.72	K	Joback Method
tc	751.37	K	Joback Method
tf	373.03	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.32	J/mol×K	553.72	Joback Method
cpg	482.50	J/mol×K	586.66	Joback Method
cpg	498.49	J/mol×K	619.60	Joback Method
cpg	513.48	J/mol×K	652.55	Joback Method
cpg	527.65	J/mol×K	685.49	Joback Method

cpg	541.19	J/mol×K	718.43	Joback Method
cpg	554.29	J/mol×K	751.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28587555&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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