

exo-Norborneol, trifluoroacetate

Other names:	Acetic acid, trifluoro-, 2-norbornyl ester, exo-
Inchi:	InChI=1S/C9H11F3O2/c10-9(11,12)8(13)14-7-4-5-1-2-6(7)3-5/h5-7H,1-4H2
InchiKey:	TYDZLCYUJXYS AI-UHFFFAOYSA-N
Formula:	C9H11F3O2
SMILES:	O=C(OC1CC2CCC1C2)C(F)(F)F
Mol. weight [g/mol]:	208.18
CAS:	31024-13-2

Physical Properties

Property code	Value	Unit	Source
gf	-688.92	kJ/mol	Joback Method
hf	-951.87	kJ/mol	Joback Method
hfus	18.92	kJ/mol	Joback Method
hvap	40.73	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.280		Crippen Method
mcvol	128.700	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	489.27	K	Joback Method
tc	679.52	K	Joback Method
tf	295.66	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.32	J/mol×K	489.27	Joback Method
cpg	337.84	J/mol×K	520.98	Joback Method
cpg	352.39	J/mol×K	552.69	Joback Method
cpg	366.01	J/mol×K	584.39	Joback Method
cpg	378.74	J/mol×K	616.10	Joback Method
cpg	390.65	J/mol×K	647.81	Joback Method
cpg	401.77	J/mol×K	679.52	Joback Method

Sources

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=C31024132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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