Crotyl alcohol, trifluoroacetate

Inchi: InChI=1S/C6H7F3O2/c1-2-3-4-11-5(10)6(7,8)9/h2-3H,4H2,1H3/b3-2+
InchiKey: XBSBZMNVXMVAHP-NSCUHMNNSA-N
Formula: C6H7F3O2
SMILES: CC=CCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 168.11

Physical Properties

Property code	Value	Unit	Source
gf	-735.65	kJ/mol	Joback Method
hf	-891.83	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	34.32	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.668		Crippen Method
mcvol	103.850	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	737.60		NIST Webbook
tb	411.71	K	Joback Method
tc	580.99	K	Joback Method
tf	228.65	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.48	J/mol×K	411.71	Joback Method
cpg	220.77	J/mol×K	439.92	Joback Method
cpg	229.57	J/mol×K	468.14	Joback Method
cpg	237.91	J/mol×K	496.35	Joback Method
cpg	245.80	J/mol×K	524.57	Joback Method
cpg	253.26	J/mol×K	552.78	Joback Method
cpg	260.31	J/mol×K	580.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352266&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
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