Crotyl alcohol, heptafluorobutyrate

Inchi: InChI=1S/C8H7F7O2/c1-2-3-4-17-5(16)6(9,10)7(11,12)8(13,14)15/h2-3H,4H2,1H3/b3-2+
InchiKey: IMXAMWCXPQCKBC-NSCUHMNNSA-N
Formula: C8H7F7O2
SMILES: CC=CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 268.13

Physical Properties

Property code	Value	Unit	Source
gf	-1492.37	kJ/mol	Joback Method
hf	-1735.05	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	32.91	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.939		Crippen Method
mcvol	139.110	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	770.70		NIST Webbook
tb	448.09	K	Joback Method
tc	602.83	K	Joback Method
tf	258.39	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.08	J/mol×K	448.09	Joback Method
cpg	340.43	J/mol×K	473.88	Joback Method
cpg	351.07	J/mol×K	499.67	Joback Method
cpg	361.03	J/mol×K	525.46	Joback Method
cpg	370.34	J/mol×K	551.25	Joback Method
cpg	379.03	J/mol×K	577.04	Joback Method
cpg	387.15	J/mol×K	602.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352264&Units=SI

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