Crotyl alcohol, pentafluoropropionate

Inchi: InChI=1S/C7H7F5O2/c1-2-3-4-14-5(13)6(8,9)7(10,11)12/h2-3H,4H2,1H3/b3-2+
InchiKey: XQTSJZNHOJRYQC-NSCUHMNNSA-N
Formula: C7H7F5O2
SMILES: CC=CCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 218.12

Physical Properties

Property code	Value	Unit	Source
gf	-1114.01	kJ/mol	Joback Method
hf	-1313.44	kJ/mol	Joback Method
hfus	17.45	kJ/mol	Joback Method
hvap	33.61	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.303		Crippen Method
mcvol	121.480	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	745.60		NIST Webbook
rinpol	745.60		NIST Webbook
tb	429.90	K	Joback Method
tc	591.49	K	Joback Method
tf	243.52	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.07	J/mol×K	429.90	Joback Method
cpg	279.55	J/mol×K	456.83	Joback Method
cpg	289.42	J/mol×K	483.76	Joback Method
cpg	298.69	J/mol×K	510.70	Joback Method
cpg	307.40	J/mol×K	537.63	Joback Method
cpg	315.58	J/mol×K	564.56	Joback Method
cpg	323.24	J/mol×K	591.49	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=U352265&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume