l-Valine, n-heptafluorobutyryl-, ethyl ester

Inchi: InChI=1S/C11H14F7NO3/c1-4-22-7(20)6(5(2)3)19-8(21)9(12,13)10(14,15)11(16,17)18/h
InchiKey: HEAQWOQEFAYBNF-UHFFFAOYSA-N
Formula: C11H14F7NO3
SMILES: CCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 341.22

Physical Properties

Property code	Value	Unit	Source
gf	-1591.74	kJ/mol	Joback Method
hf	-1983.86	kJ/mol	Joback Method
hfus	26.00	kJ/mol	Joback Method
hvap	52.03	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.523		Crippen Method
mcvol	197.230	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
tb	615.73	K	Joback Method
tc	780.94	K	Joback Method
tf	369.87	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.88	J/mol×K	615.73	Joback Method
cpg	571.23	J/mol×K	643.26	Joback Method
cpg	582.80	J/mol×K	670.80	Joback Method
cpg	593.64	J/mol×K	698.33	Joback Method
cpg	603.78	J/mol×K	725.87	Joback Method
cpg	613.27	J/mol×K	753.40	Joback Method
cpg	622.13	J/mol×K	780.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320893&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