l-Valine, n-heptafluorobutyryl-, tetradecyl ester

Inchi: InChI=1S/C23H38F7NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-34-19(32)18(17(2)3)31-2
InchiKey: ACPKOSIGENDTLE-UHFFFAOYSA-N
Formula: C23H38F7NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 509.54

Physical Properties

Property code	Value	Unit	Source
gf	-1490.70	kJ/mol	Joback Method
hf	-2231.54	kJ/mol	Joback Method
hfus	57.08	kJ/mol	Joback Method
hvap	78.75	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	7.204		Crippen Method
mcvol	366.310	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	2255.00		NIST Webbook
tb	890.29	K	Joback Method
tc	1094.53	K	Joback Method
tf	505.11	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.37	J/mol×K	890.29	Joback Method
cpg	1257.67	J/mol×K	924.33	Joback Method
cpg	1274.81	J/mol×K	958.37	Joback Method
cpg	1290.88	J/mol×K	992.41	Joback Method
cpg	1305.99	J/mol×K	1026.45	Joback Method
cpg	1320.25	J/mol×K	1060.49	Joback Method
cpg	1333.78	J/mol×K	1094.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320904&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