l-Valine, n-heptafluorobutyryl-, heptyl ester

Inchi: InChI=1S/C16H24F7NO3/c1-4-5-6-7-8-9-27-12(25)11(10(2)3)24-13(26)14(17,18)15(19,2
InchiKey: MXZVFEVXCXJNSW-UHFFFAOYSA-N
Formula: C16H24F7NO3
SMILES: CCCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 411.36

Physical Properties

Property code	Value	Unit	Source
gf	-1549.64	kJ/mol	Joback Method
hf	-2087.06	kJ/mol	Joback Method
hfus	38.95	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.474		Crippen Method
mcvol	267.680	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	1594.00		NIST Webbook
rinpol	1594.00		NIST Webbook
tb	730.13	K	Joback Method
tc	899.90	K	Joback Method
tf	426.22	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.72	J/mol×K	730.13	Joback Method
cpg	840.14	J/mol×K	758.43	Joback Method
cpg	853.69	J/mol×K	786.72	Joback Method
cpg	866.43	J/mol×K	815.02	Joback Method
cpg	878.40	J/mol×K	843.31	Joback Method
cpg	889.67	J/mol×K	871.61	Joback Method
cpg	900.26	J/mol×K	899.90	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=U320900&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