l-Valine, n-heptafluorobutyryl-, hexyl ester

Inchi: InChI=1S/C15H22F7NO3/c1-4-5-6-7-8-26-11(24)10(9(2)3)23-12(25)13(16,17)14(18,19)1
InchiKey: FYDSVYCRZSEXAA-UHFFFAOYSA-N
Formula: C15H22F7NO3
SMILES: CCCCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 397.33

Physical Properties

Property code	Value	Unit	Source
gf	-1558.06	kJ/mol	Joback Method
hf	-2066.42	kJ/mol	Joback Method
hfus	36.36	kJ/mol	Joback Method
hvap	60.94	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.084		Crippen Method
mcvol	253.590	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	1511.00		NIST Webbook
rinpol	1511.00		NIST Webbook
tb	707.25	K	Joback Method
tc	875.10	K	Joback Method
tf	414.95	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.11	J/mol×K	707.25	Joback Method
cpg	784.12	J/mol×K	735.22	Joback Method
cpg	797.28	J/mol×K	763.20	Joback Method
cpg	809.65	J/mol×K	791.17	Joback Method
cpg	821.28	J/mol×K	819.15	Joback Method
cpg	832.20	J/mol×K	847.12	Joback Method
cpg	842.47	J/mol×K	875.10	Joback Method

Sources

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=U320899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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