L-Valine, N-heptafluorobutyryl-, n-butyl ester

Other names: L-Valine, N-heptafluorobutyryl-, isobutyl ester
Inchi: InChI=1S/C13H18F7NO3/c1-4-5-6-24-9(22)8(7(2)3)21-10(23)11(14,15)12(16,17)13(18,1
InchiKey: AOFDHKDMSRIGGQ-UHFFFAOYSA-N
Formula: C13H18F7NO3
SMILES: CCCCOC(=O)C(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 369.28

Physical Properties

Property code	Value	Unit	Source
gf	-1574.90	kJ/mol	Joback Method
hf	-2025.14	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	56.49	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.303		Crippen Method
mcvol	225.410	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	1344.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1307.00		NIST Webbook
tb	661.49	K	Joback Method
tc	827.12	K	Joback Method
tf	392.41	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.12	J/mol×K	661.49	Joback Method
cpg	675.32	J/mol×K	689.10	Joback Method
cpg	687.71	J/mol×K	716.70	Joback Method
cpg	699.34	J/mol×K	744.31	Joback Method
cpg	710.26	J/mol×K	771.91	Joback Method
cpg	720.49	J/mol×K	799.52	Joback Method

cpg	730.09	J/mol×K	827.12	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=U320896&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