L-Valine, N-(2,5-ditrifluoromethylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C20H25F6NO3/c1-4-5-6-7-10-30-18(29)16(12(2)3)27-17(28)14-11-13(19(21,22

InchiKey: NQHZAVWETNFRGM-UHFFFAOYSA-N

Formula: C20H25F6NO3

SMILES: CCCCCCOC(=O)C(NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 441.41

Physical Properties

Property code	Value	Unit	Source
gf	-1230.84	kJ/mol	Joback Method
hf	-1751.17	kJ/mol	Joback Method
hfus	46.91	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	5.602		Crippen Method
mcvol	298.510	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	862.25	K	Joback Method
tc	1058.04	K	Joback Method
tf	519.75	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.71	J/mol×K	862.25	Joback Method
cpg	967.69	J/mol×K	894.88	Joback Method
cpg	980.70	J/mol×K	927.51	Joback Method
cpg	992.79	J/mol×K	960.15	Joback Method
cpg	1004.03	J/mol×K	992.78	Joback Method
cpg	1014.48	J/mol×K	1025.41	Joback Method
cpg	1024.23	J/mol×K	1058.04	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=U346572&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