L-Valine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, isohexyl ester

Inchi: InChI=1S/C19H25F4NO3/c1-11(2)7-6-10-27-18(26)16(12(3)4)24-17(25)13-8-5-9-14(15(1

InchiKey: LMGVXSICSIWZFO-UHFFFAOYSA-N

Formula: C19H25F4NO3

SMILES: CC(C)CCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1F)C(C)C

Mol. weight [g/mol]: 391.40

Physical Properties

Property code	Value	Unit	Source
gf	-854.92	kJ/mol	Joback Method
hf	-1334.84	kJ/mol	Joback Method
hfus	42.05	kJ/mol	Joback Method
hvap	78.10	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.578		Crippen Method
mcvol	280.880	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	843.62	K	Joback Method
tc	1040.84	K	Joback Method
tf	489.88	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.31	J/mol×K	843.62	Joback Method
cpg	894.64	J/mol×K	876.49	Joback Method
cpg	907.95	J/mol×K	909.36	Joback Method
cpg	920.28	J/mol×K	942.23	Joback Method
cpg	931.69	J/mol×K	975.10	Joback Method
cpg	942.22	J/mol×K	1007.97	Joback Method
cpg	951.91	J/mol×K	1040.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346466&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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