L-Valine, N-(4-fluoro-2-trifluoromethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C20H27F4NO3/c1-4-5-6-7-8-11-28-19(27)17(13(2)3)25-18(26)15-10-9-14(21)1

InchiKey: TXGAORSZQSSEPY-UHFFFAOYSA-N

Formula: C20H27F4NO3

SMILES: CCCCCCCOC(=O)C(NC(=O)c1ccc(F)cc1C(F)(F)F)C(C)C

Mol. weight [g/mol]: 405.43

Physical Properties

Property code	Value	Unit	Source
gf	-844.06	kJ/mol	Joback Method
hf	-1350.20	kJ/mol	Joback Method
hfus	48.16	kJ/mol	Joback Method
hvap	80.71	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.113		Crippen Method
mcvol	294.970	ml/mol	McGowan Method
pc	1222.55	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	866.94	K	Joback Method
tc	1065.05	K	Joback Method
tf	516.15	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.18	J/mol×K	866.94	Joback Method
cpg	952.76	J/mol×K	899.96	Joback Method
cpg	966.29	J/mol×K	932.98	Joback Method
cpg	978.85	J/mol×K	966.00	Joback Method
cpg	990.46	J/mol×K	999.02	Joback Method
cpg	1001.20	J/mol×K	1032.04	Joback Method
cpg	1011.09	J/mol×K	1065.05	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=U346483&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