L-Valine, N-(3-trifluoromethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C20H28F3NO3/c1-4-5-6-7-8-12-27-19(26)17(14(2)3)24-18(25)15-10-9-11-16(1

InchiKey: NKJPNBPZFBJGCP-UHFFFAOYSA-N

Formula: C20H28F3NO3

SMILES: CCCCCCCOC(=O)C(NC(=O)c1cccc(C(F)(F)F)c1)C(C)C

Mol. weight [g/mol]: 387.44

Physical Properties

Property code	Value	Unit	Source
gf	-639.62	kJ/mol	Joback Method
hf	-1142.62	kJ/mol	Joback Method
hfus	45.47	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	4.973		Crippen Method
mcvol	293.200	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2269.00		NIST Webbook
rinpol	2269.00		NIST Webbook
tb	862.69	K	Joback Method
tc	1062.60	K	Joback Method
tf	503.04	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	931.69	J/mol×K	862.69	Joback Method
cpg	946.65	J/mol×K	896.01	Joback Method
cpg	960.54	J/mol×K	929.33	Joback Method
cpg	973.43	J/mol×K	962.65	Joback Method
cpg	985.38	J/mol×K	995.97	Joback Method
cpg	996.44	J/mol×K	1029.28	Joback Method
cpg	1006.66	J/mol×K	1062.60	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=U346720&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