

L-Valine, N-(3-fluoro-5-trifluoromethylbenzoyl)-, propyl

Inchi:
ester

InChI=1S/C16H19F4NO3/c1-4-5-24-15(23)13(9(2)3)21-14(22)10-6-11(16(18,19)20)8-12

InchiKey:

XXMTWGXXWQWRQZ-UHFFFAOYSA-N

Formula:

C16H19F4NO3

SMILES:

CCCOC(=O)C(NC(=O)c1cc(F)cc(C(F)(F)F)c1)C(C)C

Mol. weight [g/mol]:

349.32

Physical Properties

Property code	Value	Unit	Source
gf	-877.74	kJ/mol	Joback Method
hf	-1267.64	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	71.81	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.552		Crippen Method
mvol	238.610	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	1814.00		NIST Webbook
rinpol	1814.00		NIST Webbook
tb	775.42	K	Joback Method
tc	968.98	K	Joback Method
tf	471.07	K	Joback Method
vc	0.938	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.57	J/molxK	775.42	Joback Method
cpg	722.86	J/molxK	807.68	Joback Method
cpg	735.23	J/molxK	839.94	Joback Method
cpg	746.73	J/molxK	872.20	Joback Method
cpg	757.39	J/molxK	904.46	Joback Method
cpg	767.26	J/molxK	936.72	Joback Method
cpg	776.36	J/molxK	968.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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