

D-Alanine, N-(2-fluoro-5-trifluoromethylbenzoyl)-, butyl

Inchi:
ester

InChI=1S/C15H17F4NO3/c1-3-4-7-23-14(22)9(2)20-13(21)11-8-10(15(17,18)19)5-6-12(1

InchiKey:

LNTAWAYTFDIJMF-UHFFFAOYSA-N

Formula:

C15H17F4NO3

SMILES:

CCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]:

335.29

Physical Properties

Property code	Value	Unit	Source
gf	-883.72	kJ/mol	Joback Method
hf	-1241.72	kJ/mol	Joback Method
hfus	38.74	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.306		Crippen Method
mcvol	224.520	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
tb	752.98	K	Joback Method
tc	944.62	K	Joback Method
tf	474.80	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.17	J/molxK	752.98	Joback Method
cpg	666.93	J/molxK	784.92	Joback Method
cpg	678.84	J/molxK	816.86	Joback Method
cpg	689.93	J/molxK	848.80	Joback Method
cpg	700.23	J/molxK	880.74	Joback Method
cpg	709.78	J/molxK	912.68	Joback Method
cpg	718.60	J/molxK	944.62	Joback Method

Sources

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=U348345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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