

D-Alanine, N-(3,4-difluorobenzoyl)-, hexyl ester

Inchi:	InChI=1S/C16H21F2NO3/c1-3-4-5-6-9-22-16(21)11(2)19-15(20)12-7-8-13(17)14(18)10-1
InchiKey:	HGJAGVXQBDYUOI-UHFFFAOYSA-N
Formula:	C16H21F2NO3
SMILES:	CCCCCOC(=O)C(C)NC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	313.34

Physical Properties

Property code	Value	Unit	Source
gf	-488.52	kJ/mol	Joback Method
hf	-861.39	kJ/mol	Joback Method
hfus	42.58	kJ/mol	Joback Method
hvap	75.13	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.207		Crippen Method
mcvol	235.070	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	2136.00		NIST Webbook
tb	780.55	K	Joback Method
tc	976.25	K	Joback Method
tf	482.47	K	Joback Method
vc	0.918	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.81	J/mol×K	780.55	Joback Method
cpg	705.69	J/mol×K	813.17	Joback Method
cpg	718.66	J/mol×K	845.78	Joback Method
cpg	730.73	J/mol×K	878.40	Joback Method
cpg	741.94	J/mol×K	911.02	Joback Method
cpg	752.31	J/mol×K	943.63	Joback Method
cpg	761.85	J/mol×K	976.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U348362&Units=SI

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
m cvol:	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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