

D-Alanine,
N-(3-fluoro-4-trifluoromethylbenzoyl)-, ethyl
ester

Inchi:
InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H13F4NO3/c1-3-21-12(20)7(2)18-11(19)8-4-5-9(10(14)6-8)13(15,16)17/h4
LQEPWMNNUGKCFT-UHFFFAOYSA-N
C13H13F4NO3
CCOC(=O)C(C)NC(=O)c1ccc(C(F)(F)F)c(F)c1
307.24

Physical Properties

Property code	Value	Unit	Source
gf	-900.56	kJ/mol	Joback Method
hf	-1200.44	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	65.52	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.526		Crippen Method
mcvol	196.340	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1710.00		NIST Webbook
tb	707.22	K	Joback Method
tc	900.82	K	Joback Method
tf	452.26	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.77	J/mol×K	707.22	Joback Method
cpg	559.70	J/mol×K	739.49	Joback Method
cpg	570.82	J/mol×K	771.75	Joback Method
cpg	581.17	J/mol×K	804.02	Joback Method
cpg	590.78	J/mol×K	836.29	Joback Method
cpg	599.67	J/mol×K	868.55	Joback Method
cpg	607.87	J/mol×K	900.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U347778&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
hvac:	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

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