

L-Phenylalanine, N-(3-trifluoromethylbenzoyl)-, methyl ester

Inchi:	InChI=1S/C18H16F3NO3/c1-25-17(24)15(10-12-6-3-2-4-7-12)22-16(23)13-8-5-9-14(11-1
InchiKey:	NJOHCJJTABIYRI-UHFFFAOYSA-N
Formula:	C18H16F3NO3
SMILES:	COC(=O)C(Cc1cccc1)NC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	351.32

Physical Properties

Property code	Value	Unit	Source
gf	-541.61	kJ/mol	Joback Method
hf	-859.53	kJ/mol	Joback Method
hfus	37.86	kJ/mol	Joback Method
hvap	79.08	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.219		Crippen Method
mvol	241.260	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	844.05	K	Joback Method
tc	1064.30	K	Joback Method
tf	521.92	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.35	J/molxK	844.05	Joback Method
cpg	731.65	J/molxK	880.76	Joback Method
cpg	742.86	J/molxK	917.47	Joback Method
cpg	753.07	J/molxK	954.17	Joback Method
cpg	762.35	J/molxK	990.88	Joback Method
cpg	770.78	J/molxK	1027.59	Joback Method
cpg	778.42	J/molxK	1064.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299702&Units=SI
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

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

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