

Sarcosine, n-(3-fluorobenzoyl)-, hexyl ester

Inchi:	InChI=1S/C16H22FNO3/c1-3-4-5-6-10-21-15(19)12-18(2)16(20)13-8-7-9-14(17)11-13/h7
InchiKey:	FMPYAHUESVIVFQ-UHFFFAOYSA-N
Formula:	C16H22FNO3
SMILES:	CCCCCOC(=O)CN(C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]:	295.35

Physical Properties

Property code	Value	Unit	Source
hfus	41.34	kJ/mol	Joback Method
ie	8.76	eV	Cheméo Relay (1.0)
log10ws	-3.97		Cheméo Relay (1.0)
logp	3.021		Crippen Method
mcvol	233.300	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	612.85	K	Cheméo Relay (1.0)
tf	290.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.72	J/mol×K	739.01	Joback Method
cpg	683.74	J/mol×K	771.43	Joback Method
cpg	697.82	J/mol×K	803.85	Joback Method
cpg	711.00	J/mol×K	836.28	Joback Method
cpg	723.31	J/mol×K	868.70	Joback Method
cpg	734.77	J/mol×K	901.12	Joback Method
cpg	745.43	J/mol×K	933.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321388&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point

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