Sarcosine, N-(4-fluorobenzoyl)-, heptyl ester

Inchi: InChI=1S/C17H24FNO3/c1-3-4-5-6-7-12-22-16(20)13-19(2)17(21)14-8-10-15(18)11-9-14
InchiKey: SHPXBXYWFZAGSJ-UHFFFAOYSA-N
Formula: C17H24FNO3
SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 309.38

Physical Properties

Property code	Value	Unit	Source
gf	-251.83	kJ/mol	Joback Method
hf	-655.11	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	73.50	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.411		Crippen Method
mcvol	247.390	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	2260.00		NIST Webbook
tb	761.89	K	Joback Method
tc	955.63	K	Joback Method
tf	475.44	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.57	J/mol×K	761.89	Joback Method
cpg	739.90	J/mol×K	794.18	Joback Method
cpg	754.28	J/mol×K	826.47	Joback Method
cpg	767.72	J/mol×K	858.76	Joback Method
cpg	780.27	J/mol×K	891.05	Joback Method
cpg	791.96	J/mol×K	923.34	Joback Method
cpg	802.82	J/mol×K	955.63	Joback Method

Sources

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=U321311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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