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

Inchi: InChI=1S/C16H22FNO3/c1-12(2)5-4-10-21-15(19)11-18(3)16(20)13-6-8-14(17)9-7-13/h6
InchiKey: HJOAOINBZKWCBD-UHFFFAOYSA-N
Formula: C16H22FNO3
SMILES: CC(C)CCCOC(=O)CN(C)C(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 295.35

Physical Properties

Property code	Value	Unit	Source
gf	-262.69	kJ/mol	Joback Method
hf	-639.75	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	70.89	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.877		Crippen Method
mcvol	233.300	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	738.57	K	Joback Method
tc	935.79	K	Joback Method
tf	449.17	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.25	J/mol×K	738.57	Joback Method
cpg	684.49	J/mol×K	771.44	Joback Method
cpg	698.76	J/mol×K	804.31	Joback Method
cpg	712.09	J/mol×K	837.18	Joback Method
cpg	724.52	J/mol×K	870.05	Joback Method
cpg	736.07	J/mol×K	902.92	Joback Method
cpg	746.78	J/mol×K	935.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321310&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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