Sarcosine, N-(2-fluorobenzoyl)-, decyl ester

Inchi: InChI=1S/C20H30FNO3/c1-3-4-5-6-7-8-9-12-15-25-19(23)16-22(2)20(24)17-13-10-11-14
InchiKey: GQFJOLDNCFKLEE-UHFFFAOYSA-N
Formula: C20H30FNO3
SMILES: CCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1F
Mol. weight [g/mol]: 351.46

Physical Properties

Property code	Value	Unit	Source
gf	-226.57	kJ/mol	Joback Method
hf	-717.03	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	80.18	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.582		Crippen Method
mcvol	289.660	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	2572.00		NIST Webbook
rinpol	2572.00		NIST Webbook
tb	830.53	K	Joback Method
tc	1025.47	K	Joback Method
tf	509.25	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.87	J/mol×K	830.53	Joback Method
cpg	914.05	J/mol×K	863.02	Joback Method
cpg	929.19	J/mol×K	895.51	Joback Method
cpg	943.31	J/mol×K	928.00	Joback Method
cpg	956.47	J/mol×K	960.49	Joback Method
cpg	968.70	J/mol×K	992.98	Joback Method
cpg	980.04	J/mol×K	1025.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321248&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
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

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