Sarcosine, N-(3-bromobenzoyl)-, dodecyl ester

Inchi: InChI=1S/C22H34BrNO3/c1-3-4-5-6-7-8-9-10-11-12-16-27-21(25)18-24(2)22(26)19-14-1
InchiKey: VPWIQHAIDKKLRJ-UHFFFAOYSA-N
Formula: C22H34BrNO3
SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 440.41

Physical Properties

Property code	Value	Unit	Source
gf	-0.60	kJ/mol	Joback Method
hf	-535.87	kJ/mol	Joback Method
hfus	59.08	kJ/mol	Joback Method
hvap	91.88	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.985		Crippen Method
mcvol	333.570	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	3266.00		NIST Webbook
rinpol	3266.00		NIST Webbook
tb	943.18	K	Joback Method
tc	1157.35	K	Joback Method
tf	591.00	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1052.13	J/mol×K	943.18	Joback Method
cpg	1067.71	J/mol×K	978.87	Joback Method
cpg	1082.17	J/mol×K	1014.57	Joback Method
cpg	1095.58	J/mol×K	1050.26	Joback Method
cpg	1108.01	J/mol×K	1085.96	Joback Method
cpg	1119.53	J/mol×K	1121.65	Joback Method
cpg	1130.19	J/mol×K	1157.35	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=U321185&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