

Sarcosine, N-(2-bromobenzoyl)-, tetradecyl ester

Inchi:	InChI=1S/C24H38BrNO3/c1-3-4-5-6-7-8-9-10-11-12-13-16-19-29-23(27)20-26(2)24(28)2
InchiKey:	IZNDKTAEMSJHHD-UHFFFAOYSA-N
Formula:	C24H38BrNO3
SMILES:	CCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]:	468.47

Physical Properties

Property code	Value	Unit	Source
gf	16.24	kJ/mol	Joback Method
hf	-577.15	kJ/mol	Joback Method
hfus	64.26	kJ/mol	Joback Method
hvap	96.34	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.765		Crippen Method
mcvol	361.750	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
tb	988.94	K	Joback Method
tc	1210.78	K	Joback Method
tf	613.54	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.59	J/molxK	988.94	Joback Method
cpg	1190.84	J/molxK	1025.91	Joback Method
cpg	1205.88	J/molxK	1062.89	Joback Method
cpg	1219.81	J/molxK	1099.86	Joback Method
cpg	1232.70	J/molxK	1136.83	Joback Method
cpg	1244.64	J/molxK	1173.81	Joback Method
cpg	1255.70	J/molxK	1210.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U321460&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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