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

Inchi: InChI=1S/C21H32BrNO3/c1-3-4-5-6-7-8-9-10-11-15-26-20(24)17-23(2)21(25)18-13-12-1
InchiKey: OZKKLMOJSXGVBA-UHFFFAOYSA-N
Formula: C21H32BrNO3
SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 426.39

Physical Properties

Property code	Value	Unit	Source
gf	-9.02	kJ/mol	Joback Method
hf	-515.23	kJ/mol	Joback Method
hfus	56.49	kJ/mol	Joback Method
hvap	89.66	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.595		Crippen Method
mcvol	319.480	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	3083.00		NIST Webbook
tb	920.30	K	Joback Method
tc	1132.03	K	Joback Method
tf	579.73	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.80	J/mol×K	920.30	Joback Method
cpg	1007.10	J/mol×K	955.59	Joback Method
cpg	1021.31	J/mol×K	990.88	Joback Method
cpg	1034.49	J/mol×K	1026.17	Joback Method
cpg	1046.71	J/mol×K	1061.46	Joback Method
cpg	1058.04	J/mol×K	1096.74	Joback Method
cpg	1068.53	J/mol×K	1132.03	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=U321184&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