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

Inchi: InChI=1S/C20H30BrNO3/c1-3-4-5-6-7-8-9-12-15-25-19(23)16-22(2)20(24)17-13-10-11-1
InchiKey: LSAOGMWTHDGDRK-UHFFFAOYSA-N
Formula: C20H30BrNO3
SMILES: CCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 412.36

Physical Properties

Property code	Value	Unit	Source
gf	-17.44	kJ/mol	Joback Method
hf	-494.59	kJ/mol	Joback Method
hfus	53.90	kJ/mol	Joback Method
hvap	87.43	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.205		Crippen Method
mcvol	305.390	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2874.00		NIST Webbook
rinpol	2874.00		NIST Webbook
tb	897.42	K	Joback Method
tc	1107.57	K	Joback Method
tf	568.46	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.14	J/mol×K	897.42	Joback Method
cpg	947.17	J/mol×K	932.44	Joback Method
cpg	961.14	J/mol×K	967.47	Joback Method
cpg	974.11	J/mol×K	1002.49	Joback Method
cpg	986.14	J/mol×K	1037.52	Joback Method
cpg	997.28	J/mol×K	1072.54	Joback Method
cpg	1007.60	J/mol×K	1107.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321457&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