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

Inchi: InChI=1S/C12H14BrNO3/c1-3-17-11(15)8-14(2)12(16)9-6-4-5-7-10(9)13/h4-7H,3,8H2,1-
InchiKey: FQPKGVVKAKLULP-UHFFFAOYSA-N
Formula: C12H14BrNO3
SMILES: CCOC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 300.15

Physical Properties

Property code	Value	Unit	Source
gf	-84.80	kJ/mol	Joback Method
hf	-329.47	kJ/mol	Joback Method
hfus	33.18	kJ/mol	Joback Method
hvap	69.62	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.084		Crippen Method
mcvol	192.670	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	2019.00		NIST Webbook
tb	714.38	K	Joback Method
tc	936.36	K	Joback Method
tf	478.30	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.82	J/mol×K	714.38	Joback Method
cpg	498.31	J/mol×K	751.38	Joback Method
cpg	509.88	J/mol×K	788.37	Joback Method
cpg	520.58	J/mol×K	825.37	Joback Method
cpg	530.45	J/mol×K	862.36	Joback Method
cpg	539.52	J/mol×K	899.36	Joback Method
cpg	547.84	J/mol×K	936.36	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=U321448&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

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