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

Inchi: InChI=1S/C13H16BrNO3/c1-3-8-18-12(16)9-15(2)13(17)10-6-4-5-7-11(10)14/h4-7H,3,8-9
InchiKey: ZXRWTTKRDIRKHP-UHFFFAOYSA-N
Formula: C13H16BrNO3
SMILES: CCCOC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 314.18

Physical Properties

Property code	Value	Unit	Source
gf	-76.38	kJ/mol	Joback Method
hf	-350.11	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.474		Crippen Method
mcvol	206.760	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	2119.00		NIST Webbook
rinpol	2119.00		NIST Webbook
tb	737.26	K	Joback Method
tc	955.80	K	Joback Method
tf	489.57	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.98	J/mol×K	737.26	Joback Method
cpg	550.93	J/mol×K	773.68	Joback Method
cpg	562.95	J/mol×K	810.11	Joback Method
cpg	574.07	J/mol×K	846.53	Joback Method
cpg	584.35	J/mol×K	882.95	Joback Method
cpg	593.81	J/mol×K	919.38	Joback Method
cpg	602.50	J/mol×K	955.80	Joback Method

Sources

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=U321449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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