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

Inchi: InChI=1S/C14H18BrNO3/c1-10(2)9-19-13(17)8-16(3)14(18)11-6-4-5-7-12(11)15/h4-7,10
InchiKey: HNYJWBWORKAODO-UHFFFAOYSA-N
Formula: C14H18BrNO3
SMILES: CC(C)COC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 328.20

Physical Properties

Property code	Value	Unit	Source
gf	-70.40	kJ/mol	Joback Method
hf	-376.03	kJ/mol	Joback Method
hfus	34.84	kJ/mol	Joback Method
hvap	73.69	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.720		Crippen Method
mcvol	220.850	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
tb	759.70	K	Joback Method
tc	978.79	K	Joback Method
tf	485.84	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.91	J/mol×K	759.70	Joback Method
cpg	605.47	J/mol×K	796.21	Joback Method
cpg	618.05	J/mol×K	832.73	Joback Method
cpg	629.67	J/mol×K	869.24	Joback Method
cpg	640.40	J/mol×K	905.76	Joback Method
cpg	650.26	J/mol×K	942.27	Joback Method
cpg	659.31	J/mol×K	978.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321450&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