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

Inchi: InChI=1S/C14H18BrNO3/c1-3-4-8-19-13(17)10-16(2)14(18)11-6-5-7-12(15)9-11/h5-7,9H
InchiKey: GJKOYCPJMZZHNB-UHFFFAOYSA-N
Formula: C14H18BrNO3
SMILES: CCCCOC(=O)CN(C)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 328.20

Physical Properties

Property code	Value	Unit	Source
gf	-67.96	kJ/mol	Joback Method
hf	-370.75	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	74.08	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.864		Crippen Method
mcvol	220.850	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	2263.00		NIST Webbook
tb	760.14	K	Joback Method
tc	975.72	K	Joback Method
tf	500.84	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.33	J/mol×K	760.14	Joback Method
cpg	604.67	J/mol×K	796.07	Joback Method
cpg	617.07	J/mol×K	832.00	Joback Method
cpg	628.55	J/mol×K	867.93	Joback Method
cpg	639.18	J/mol×K	903.86	Joback Method
cpg	648.98	J/mol×K	939.79	Joback Method
cpg	658.00	J/mol×K	975.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321179&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

Latest version available from:
https://www.chemeo.com/cid/44-685-3/Sarcosine-N-3-bromobenzoyl-butyl-ester.pdf
Generated by Cheméo on 2024-04-27 10:27:15.279720181 +0000 UTC m=+16502884.200297502.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.