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]: 328.21

Physical Properties

Property code	Value	Unit	Source
af	0.7381		Cheméo Relay (1.0)
hfus	38.36	kJ/mol	Joback Method
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-3.91		Cheméo Relay (1.0)
logp	2.864		Crippen Method
mcvol	220.850	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	2263.00		NIST Webbook
tb	624.85	K	Cheméo Relay (1.0)
tc	832.64	K	Cheméo Relay (1.0)
tf	300.03	K	Cheméo Relay (1.0)
vc	0.791	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321179&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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