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

Inchi: InChI=1S/C16H22BrNO3/c1-3-4-5-8-11-21-15(19)12-18(2)16(20)13-9-6-7-10-14(13)17/h
InchiKey: QVCVUHLWKOENSG-UHFFFAOYSA-N
Formula: C16H22BrNO3
SMILES: CCCCCCOC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 356.25

Physical Properties

Property code	Value	Unit	Source
gf	-51.12	kJ/mol	Joback Method
hf	-412.03	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	78.53	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.645		Crippen Method
mcvol	249.030	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2425.00		NIST Webbook
rinpol	2425.00		NIST Webbook
tb	805.90	K	Joback Method
tc	1017.15	K	Joback Method
tf	523.38	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.25	J/mol×K	805.90	Joback Method
cpg	715.25	J/mol×K	841.11	Joback Method
cpg	728.26	J/mol×K	876.32	Joback Method
cpg	740.33	J/mol×K	911.52	Joback Method
cpg	751.52	J/mol×K	946.73	Joback Method
cpg	761.86	J/mol×K	981.94	Joback Method
cpg	771.41	J/mol×K	1017.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321454&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