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

Inchi: InChI=1S/C17H24BrNO3/c1-3-4-5-6-9-12-22-16(20)13-19(2)17(21)14-10-7-8-11-15(14)1
InchiKey: UIPDVBGFJZCDLH-UHFFFAOYSA-N
Formula: C17H24BrNO3
SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 370.28

Physical Properties

Property code	Value	Unit	Source
gf	-42.70	kJ/mol	Joback Method
hf	-432.67	kJ/mol	Joback Method
hfus	46.13	kJ/mol	Joback Method
hvap	80.75	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.035		Crippen Method
mcvol	263.120	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook
tb	828.78	K	Joback Method
tc	1038.74	K	Joback Method
tf	534.65	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.69	J/mol×K	828.78	Joback Method
cpg	771.96	J/mol×K	863.77	Joback Method
cpg	785.23	J/mol×K	898.77	Joback Method
cpg	797.55	J/mol×K	933.76	Joback Method
cpg	808.97	J/mol×K	968.75	Joback Method
cpg	819.54	J/mol×K	1003.74	Joback Method
cpg	829.30	J/mol×K	1038.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321455&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