Sarcosine, N-(4-bromobenzoyl)-, octyl ester

Inchi: InChI=1S/C18H26BrNO3/c1-3-4-5-6-7-8-13-23-17(21)14-20(2)18(22)15-9-11-16(19)12-1
InchiKey: ABCWLUUEOCOVOE-UHFFFAOYSA-N
Formula: C18H26BrNO3
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 384.31

Physical Properties

Property code	Value	Unit	Source
gf	-34.28	kJ/mol	Joback Method
hf	-453.31	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	82.98	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.425		Crippen Method
mcvol	277.210	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2682.00		NIST Webbook
tb	851.66	K	Joback Method
tc	1060.97	K	Joback Method
tf	545.92	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.03	J/mol×K	851.66	Joback Method
cpg	829.55	J/mol×K	886.55	Joback Method
cpg	843.06	J/mol×K	921.43	Joback Method
cpg	855.61	J/mol×K	956.32	Joback Method
cpg	867.24	J/mol×K	991.20	Joback Method
cpg	878.01	J/mol×K	1026.09	Joback Method
cpg	887.97	J/mol×K	1060.97	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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