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

Inchi: InChI=1S/C15H20BrNO3/c1-3-4-7-10-20-14(18)11-17(2)15(19)12-8-5-6-9-13(12)16/h5-6
InchiKey: ZKGHCIKFIPTLSN-UHFFFAOYSA-N
Formula: C15H20BrNO3
SMILES: CCCCCOC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 342.23

Physical Properties

Property code	Value	Unit	Source
gf	-59.54	kJ/mol	Joback Method
hf	-391.39	kJ/mol	Joback Method
hfus	40.95	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.254		Crippen Method
mcvol	234.940	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	783.02	K	Joback Method
tc	996.16	K	Joback Method
tf	512.11	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.77	J/mol×K	783.02	Joback Method
cpg	659.46	J/mol×K	818.54	Joback Method
cpg	672.19	J/mol×K	854.07	Joback Method
cpg	683.99	J/mol×K	889.59	Joback Method
cpg	694.91	J/mol×K	925.11	Joback Method
cpg	705.00	J/mol×K	960.63	Joback Method
cpg	714.30	J/mol×K	996.16	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=U321452&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