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

Inchi: InChI=1S/C16H22BrNO3/c1-12(2)5-4-10-21-15(19)11-18(3)16(20)13-6-8-14(17)9-7-13/h

InchiKey: JCLOXHDIHPJQAH-UHFFFAOYSA-N

Formula: C16H22BrNO3

SMILES: CC(C)CCCOC(=O)CN(C)C(=O)c1ccc(Br)cc1

Mol. weight [g/mol]: 356.25

Physical Properties

Property code	Value	Unit	Source
gf	-53.56	kJ/mol	Joback Method
hf	-417.31	kJ/mol	Joback Method
hfus	40.02	kJ/mol	Joback Method
hvap	78.14	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.501		Crippen Method
mcvol	249.030	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	2429.00		NIST Webbook
rinpol	2429.00		NIST Webbook
tb	805.46	K	Joback Method
tc	1019.60	K	Joback Method
tf	508.38	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.82	J/mol×K	805.46	Joback Method
cpg	716.00	J/mol×K	841.15	Joback Method
cpg	729.15	J/mol×K	876.84	Joback Method
cpg	741.34	J/mol×K	912.53	Joback Method
cpg	752.60	J/mol×K	948.22	Joback Method
cpg	762.99	J/mol×K	983.91	Joback Method
cpg	772.54	J/mol×K	1019.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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