

Sarcosine, N-(3-bromobenzoyl)-, nonyl ester

Inchi: InChI=1S/C19H28BrNO3/c1-3-4-5-6-7-8-9-13-24-18(22)15-21(2)19(23)16-11-10-12-17(2)
InchiKey: QMBQQYUDQJCHAT-UHFFFAOYSA-N
Formula: C19H28BrNO3
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 398.33

Physical Properties

Property code	Value	Unit	Source
gf	-25.86	kJ/mol	Joback Method
hf	-473.95	kJ/mol	Joback Method
hfus	51.31	kJ/mol	Joback Method
hvap	85.21	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.815		Crippen Method
mcvol	291.300	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	2786.00		NIST Webbook
rinpol	2786.00		NIST Webbook
tb	874.54	K	Joback Method
tc	1083.90	K	Joback Method
tf	557.19	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.20	J/mol×K	874.54	Joback Method
cpg	887.98	J/mol×K	909.43	Joback Method
cpg	901.72	J/mol×K	944.33	Joback Method
cpg	914.47	J/mol×K	979.22	Joback Method
cpg	926.31	J/mol×K	1014.11	Joback Method
cpg	937.27	J/mol×K	1049.01	Joback Method
cpg	947.41	J/mol×K	1083.90	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=U321183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvac:	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

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