

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

Inchi:	InChI=1S/C12H14BrNO3/c1-3-17-11(15)8-14(2)12(16)9-5-4-6-10(13)7-9/h4-7H,3,8H2,1-
InchiKey:	OZECLKHTCCASLT-UHFFFAOYSA-N
Formula:	C12H14BrNO3
SMILES:	CCOC(=O)CN(C)C(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	300.15

Physical Properties

Property code	Value	Unit	Source
gf	-84.80	kJ/mol	Joback Method
hf	-329.47	kJ/mol	Joback Method
hfus	33.18	kJ/mol	Joback Method
hvap	69.62	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.084		Crippen Method
mcvol	192.670	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpola	2068.00		NIST Webbook
rinpola	2068.00		NIST Webbook
tb	714.38	K	Joback Method
tc	936.36	K	Joback Method
tf	478.30	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.82	J/molxK	714.38	Joback Method
cpg	498.31	J/molxK	751.38	Joback Method
cpg	509.88	J/molxK	788.37	Joback Method
cpg	520.58	J/molxK	825.37	Joback Method
cpg	530.45	J/molxK	862.36	Joback Method
cpg	539.52	J/molxK	899.36	Joback Method
cpg	547.84	J/molxK	936.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/122-831-3/Sarcosine-N-3-bromobenzoyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-27 10:35:33.925411709 +0000 UTC m=+16503382.845989022.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.