

Butanilicaine

Other names:	2-(Butylamino)-6'-chloro-o-acetoluidide Butacetoluide 2-(Butylamino)-6'-chloro-o-acetotoluidide
Inchi:	InChI=1S/C13H19ClN2O/c1-3-4-8-15-9-12(17)16-13-10(2)6-5-7-11(13)14/h5-7,15H,3-4,8
InchiKey:	VWYQKFLGRBICZ-UHFFFAOYSA-N
Formula:	C13H19ClN2O
SMILES:	CCCCNCC(=O)Nc1c(C)cccc1Cl
Mol. weight [g/mol]:	254.76
CAS:	3785-21-5

Physical Properties

Property code	Value	Unit	Source
gf	189.66	kJ/mol	Joback Method
hf	-119.44	kJ/mol	Joback Method
hfus	38.68	kJ/mol	Joback Method
hvap	72.13	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.977		Crippen Method
mcvol	204.040	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	725.12	K	Joback Method
tc	935.26	K	Joback Method
tf	472.90	K	Joback Method
vc	0.780	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.74	J/molxK	725.12	Joback Method

cpg	563.57	J/mol×K	760.14	Joback Method
cpg	576.52	J/mol×K	795.17	Joback Method
cpg	588.62	J/mol×K	830.19	Joback Method
cpg	599.92	J/mol×K	865.21	Joback Method
cpg	610.44	J/mol×K	900.24	Joback Method
cpg	620.22	J/mol×K	935.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3785215&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:

<https://www.chemeo.com/cid/123-927-6/Butanilicaine.pdf>

Generated by Cheméo on 2024-04-29 16:59:10.971092363 +0000 UTC m=+16699199.891669684.

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