

Trichlamide

Other names:

N-(1-Butoxy-2,2,2-trichloroethyl)salicylamide
WL 105305
N-(1-Butoxy-2,2,2-trichloroethyl)-2-hydroxybenzamide
NK 483
Hataclean
Benzamide, N-(1-butoxy-2,2,2-trichloroethyl)-2-hydroxy-

Inchi: InChI=1S/C13H16Cl3NO3/c1-2-3-8-20-12(13(14,15)16)17-11(19)9-6-4-5-7-10(9)18/h4-7**InchiKey:** NHTFLYKPEGXOAN-UHFFFAOYSA-N**Formula:** C13H16Cl3NO3**SMILES:** CCCCOCC(=O)Nc1ccccc1OC(Cl)(Cl)Cl**Mol. weight [g/mol]:** 340.63**CAS:** 70193-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-163.55	kJ/mol	Joback Method
hf	-505.01	kJ/mol	Joback Method
hfus	38.79	kJ/mol	Joback Method
hvap	86.88	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.635		Crippen Method
mcvol	230.280	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		NIST Webbook
ripol	3151.00		NIST Webbook
ripol	3151.00		NIST Webbook
tb	839.22	K	Joback Method
tc	1073.60	K	Joback Method
tf	576.41	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.76	J/mol×K	839.22	Joback Method
cpg	633.92	J/mol×K	878.28	Joback Method
cpg	644.44	J/mol×K	917.35	Joback Method
cpg	654.44	J/mol×K	956.41	Joback Method
cpg	664.04	J/mol×K	995.47	Joback Method
cpg	673.37	J/mol×K	1034.54	Joback Method
cpg	682.55	J/mol×K	1073.60	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=C70193214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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