

Trichlamide, N-trifluoroacetyl-

Inchi:	InChI=1S/C15H15Cl3F3NO4/c1-2-3-8-25-12(14(16,17)18)22-11(23)9-6-4-5-7-10(9)26-13
InchiKey:	BSAJPCLSGVXCLZ-UHFFFAOYSA-N
Formula:	C15H15Cl3F3NO4
SMILES:	CCCCOC(=O)c1ccccc1OC(=O)C(F)(F)F)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	436.64

Physical Properties

Property code	Value	Unit	Source
gf	-817.23	kJ/mol	Joback Method
hf	-1222.33	kJ/mol	Joback Method
hfus	42.41	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.397		Crippen Method
mvol	265.340	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook
tb	880.21	K	Joback Method
tc	1095.86	K	Joback Method
tf	576.10	K	Joback Method
vc	1.024	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.88	J/mol×K	880.21	Joback Method
cpg	753.65	J/mol×K	916.15	Joback Method
cpg	762.52	J/mol×K	952.09	Joback Method
cpg	770.55	J/mol×K	988.04	Joback Method
cpg	777.82	J/mol×K	1023.98	Joback Method
cpg	784.38	J/mol×K	1059.92	Joback Method
cpg	790.30	J/mol×K	1095.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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