

Trichlamide, N-pentafluoropropionyl-

Inchi:	InChI=1S/C16H15Cl3F5NO4/c1-2-3-8-28-12(15(17,18)19)25-11(26)9-6-4-5-7-10(9)29-13
InchiKey:	GHRNNYVDPNBINL-UHFFFAOYSA-N
Formula:	C16H15Cl3F5NO4
SMILES:	CCCCOC(=O)c1ccccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	486.65

Physical Properties

Property code	Value	Unit	Source
gf	-1195.59	kJ/mol	Joback Method
hf	-1643.94	kJ/mol	Joback Method
hfus	43.75	kJ/mol	Joback Method
hvap	83.69	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.032		Crippen Method
mcvol	282.970	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2092.00		NIST Webbook
tb	898.40	K	Joback Method
tc	1110.35	K	Joback Method
tf	590.97	K	Joback Method
vc	1.105	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.15	J/mol×K	898.40	Joback Method
cpg	824.63	J/mol×K	933.72	Joback Method
cpg	833.28	J/mol×K	969.05	Joback Method
cpg	841.20	J/mol×K	1004.37	Joback Method
cpg	848.47	J/mol×K	1039.70	Joback Method
cpg	855.18	J/mol×K	1075.02	Joback Method
cpg	861.42	J/mol×K	1110.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374334&Units=SI

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
m cvol:	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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