

Trichlamide, N-heptafluorobutyryl-

Inchi:	InChI=1S/C17H15Cl3F7NO4/c1-2-3-8-31-12(15(18,19)20)28-11(29)9-6-4-5-7-10(9)32-13
InchiKey:	YRFYDFMPNIGBNE-UHFFFAOYSA-N
Formula:	C17H15Cl3F7NO4
SMILES:	CCCCOC(NC(=O)c1cccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	536.65

Physical Properties

Property code	Value	Unit	Source
gf	-1573.95	kJ/mol	Joback Method
hf	-2065.55	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	82.99	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	5.668		Crippen Method
mcvol	300.600	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
rinpol	2111.00		NIST Webbook
tb	916.59	K	Joback Method
tc	1126.93	K	Joback Method
tf	605.84	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.51	J/molxK	916.59	Joback Method
cpg	895.81	J/molxK	951.65	Joback Method
cpg	904.38	J/molxK	986.70	Joback Method
cpg	912.31	J/molxK	1021.76	Joback Method
cpg	919.73	J/molxK	1056.82	Joback Method
cpg	926.75	J/molxK	1091.88	Joback Method
cpg	933.48	J/molxK	1126.93	Joback Method

Sources

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=U374335&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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