

1-[1-(1-Propoxypropoxy)propoxy]propan-1-ol, pentafluoropropionate

Inchi:	InChI=1S/C15H25F5O5/c1-5-9-22-10(6-2)23-11(7-3)24-12(8-4)25-13(21)14(16,17)15(18)
InchiKey:	YXSUJVVIDZMQAN-UHFFFAOYSA-N
Formula:	C15H25F5O5
SMILES:	CCCOC(CC)OC(CC)OC(CC)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	380.35

Physical Properties

Property code	Value	Unit	Source
gf	-1449.19	kJ/mol	Joback Method
hf	-2008.28	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	57.53	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.395		Crippen Method
mvol	256.110	ml/mol	McGowan Method
pc	1252.15	kPa	Joback Method
rinpol	1430.00		NIST Webbook
rinpol	1430.00		NIST Webbook
tb	674.72	K	Joback Method
tc	838.08	K	Joback Method
tf	360.45	K	Joback Method
vc	1.004	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.68	J/mol×K	674.72	Joback Method
cpg	772.45	J/mol×K	701.95	Joback Method
cpg	787.42	J/mol×K	729.17	Joback Method
cpg	801.62	J/mol×K	756.40	Joback Method
cpg	815.05	J/mol×K	783.63	Joback Method
cpg	827.73	J/mol×K	810.85	Joback Method
cpg	839.67	J/mol×K	838.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U378345&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
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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