

2-[2-(2,2,3,3,3-Pentafluoropropanoyl)oxyethoxy]ethane

Other names: 8,8,9,9,9-Pentafluoro-7-oxo-3,6-dioxanon-1-yl pentafluoropropionate
2,2,3,3,3-pentafluoropropanoate
Diethylene glycol, bis(pentafluoropropionate)

Inchi: InChI=1S/C10H8F10O5/c11-7(12,9(15,16)17)5(21)24-3-1-23-2-4-25-6(22)8(13,14)10(18,

InchiKey: DBFSAUJMJDNLIU-UHFFFAOYSA-N

Formula: C10H8F10O5

SMILES: O=C(OCCOCCOC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 398.15

Physical Properties

Property code	Value	Unit	Source
gf	-2476.26	kJ/mol	Joback Method
hf	-2867.65	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.485		Crippen Method
mcvol	190.210	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	1030.40		NIST Webbook
rinpol	1030.40		NIST Webbook
tb	582.98	K	Joback Method
tc	731.98	K	Joback Method
tf	384.59	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.12	J/molxK	582.98	Joback Method
cpg	546.64	J/molxK	607.81	Joback Method
cpg	556.53	J/molxK	632.65	Joback Method
cpg	565.81	J/molxK	657.48	Joback Method
cpg	574.51	J/molxK	682.31	Joback Method
cpg	582.65	J/molxK	707.15	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=U352000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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