

2-[2-[2-(2,2,3,3,3-Pentafluoropropanoyl)oxyethoxy]oxy]oxy-1,1,1,1,2,12,12-Pentafluoro-10-oxo-3,6,9-trioxadodec-1-yl pentafluoropropanoate

2,2,3,3,3-pentafluoropropanoate

Other names: Triethylene glycol, bis(pentafluoropropanoate)

Inchi: InChI=1S/C12H12F10O6/c13-9(14,11(17,18)19)7(23)27-5-3-25-1-2-26-4-6-28-8(24)10(11,12)

InchiKey: FFMBKAQEBJRQCN-UHFFFAOYSA-N

Formula: C₁₂H₁₂F₁₀O₆

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

Mol. weight [g/mol]: 442.20

Physical Properties

Property code	Value	Unit	Source
gf	-2564.42	kJ/mol	Joback Method
hf	-3041.15	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.501		Crippen Method
mcvol	224.260	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	1258.80		NIST Webbook
rinpol	1258.80		NIST Webbook
tb	651.16	K	Joback Method
tc	804.85	K	Joback Method
tf	429.36	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.12	J/mol×K	651.16	Joback Method
cpg	673.51	J/mol×K	676.78	Joback Method
cpg	684.22	J/mol×K	702.39	Joback Method
cpg	694.28	J/mol×K	728.01	Joback Method
cpg	703.71	J/mol×K	753.62	Joback Method
cpg	712.53	J/mol×K	779.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351999&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
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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