2-[2-(2,2,3,3,4,4,4-Heptafluorobutanoyl)oxyethoxy]ethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Othernames: 8,8,9,9,10,10,10-Heptafluoro-7-oxo-3,6-dioxadec-1-yl Heptafluorobutyrate
Diethylene glycol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C12H8F14O5/c13-7(14,9(17,18)11(21,22)23)5(27)30-3-1-29-2-4-31-6(28)8(15,

InchiKey: BEEXQHZRCIFGJK-UHFFFAOYSA-N

Formula: C12H8F14O5

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

Mol. weight [g/mol]: 498.17

Physical Properties

Property code	Value	Unit	Source
gf	-3232.98	kJ/mol	Joback Method
hf	-3710.87	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	43.81	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.755		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	1106.60		NIST Webbook
rinpol	1106.60		NIST Webbook
tb	619.36	K	Joback Method
tc	765.02	K	Joback Method
tf	414.33	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.09	J/mol×K	619.36	Joback Method
cpg	684.99	J/mol×K	643.64	Joback Method
cpg	695.14	J/mol×K	667.91	Joback Method
cpg	704.58	J/mol×K	692.19	Joback Method
cpg	713.36	J/mol×K	716.47	Joback Method
cpg	721.50	J/mol×K	740.74	Joback Method

cpg	729.06	J/mol×K	765.02	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=U352031&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
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