2-[2-(2-Ethoxyethoxy)ethoxy]ethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Other names: Triethylene glycol monoethyl ether, heptafluorobutyrate
3,6,9-Trioxaundec-1-yl heptafluorobutyrate

Inchi: InChI=1S/C12H17F7O5/c1-2-21-3-4-22-5-6-23-7-8-24-9(20)10(13,14)11(15,16)12(17,18)

InchiKey: IMIBMDPKWPTZHS-UHFFFAOYSA-N

Formula: C12H17F7O5

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

Mol. weight [g/mol]: 374.25

Physical Properties

Property code	Value	Unit	Source
gf	-1853.91	kJ/mol	Joback Method
hf	-2331.49	kJ/mol	Joback Method
hfus	32.50	kJ/mol	Joback Method
hvap	49.09	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.432		Crippen Method
mcvol	217.380	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	1327.50		NIST Webbook
tb	602.71	K	Joback Method
tc	754.24	K	Joback Method
tf	375.24	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.27	J/mol×K	602.71	Joback Method
cpg	626.47	J/mol×K	627.97	Joback Method
cpg	639.03	J/mol×K	653.22	Joback Method
cpg	650.97	J/mol×K	678.48	Joback Method
cpg	662.31	J/mol×K	703.73	Joback Method
cpg	673.05	J/mol×K	728.99	Joback Method
cpg	683.23	J/mol×K	754.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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