

2-[2-(2-Butoxyethoxy)ethoxy]ethyl 2,2,2-trifluoroacetate

Other names:	Triethylene glycol monobutyl ether, trifluoroacetate 3,6,9-Trioxatridec-1-yl trifluoroacetate
Inchi:	InChI=1S/C12H21F3O5/c1-2-3-4-17-5-6-18-7-8-19-9-10-20-11(16)12(13,14)15/h2-10H2,
InchiKey:	UWKAFJGNHCNKJN-UHFFFAOYSA-N
Formula:	C12H21F3O5
SMILES:	CCCCOCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	302.29

Physical Properties

Property code	Value	Unit	Source
gf	-1080.35	kJ/mol	Joback Method
hf	-1529.55	kJ/mol	Joback Method
hfus	35.01	kJ/mol	Joback Method
hvap	54.95	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.942		Crippen Method
mcvol	210.300	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	1445.70		NIST Webbook
rinpol	1475.90		NIST Webbook
rinpol	1445.70		NIST Webbook
rinpol	1475.90		NIST Webbook
tb	612.09	K	Joback Method
tc	771.51	K	Joback Method
tf	368.04	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.13	J/molxK	612.09	Joback Method
cpg	589.22	J/molxK	638.66	Joback Method
cpg	602.75	J/molxK	665.23	Joback Method
cpg	615.71	J/molxK	691.80	Joback Method

cpg	628.10	J/mol×K	718.37	Joback Method
cpg	639.91	J/mol×K	744.94	Joback Method
cpg	651.16	J/mol×K	771.51	Joback Method

Sources

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=U351936&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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