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

Othernames: Pentaethylene glycol monobutyl ether, trifluoroacetate
3,6,9,12,15-Pentaoxanonadec-1-yl trifluoroacetate

Inchi: InChI=1S/C16H29F3O7/c1-2-3-4-21-5-6-22-7-8-23-9-10-24-11-12-25-13-14-26-15(20)16

InchiKey: DMZIVFFCOLMBTC-UHFFFAOYSA-N

Formula: C16H29F3O7

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

Mol. weight [g/mol]: 390.39

Physical Properties

Property code	Value	Unit	Source
gf	-1256.67	kJ/mol	Joback Method
hf	-1876.55	kJ/mol	Joback Method
hfus	47.75	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.975		Crippen Method
mcvol	278.400	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	1959.30		NIST Webbook
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook
rinpol	1959.30		NIST Webbook
tb	748.45	K	Joback Method
tc	918.48	K	Joback Method
tf	457.58	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.07	J/mol×K	748.45	Joback Method
cpg	871.27	J/mol×K	776.79	Joback Method
cpg	886.60	J/mol×K	805.13	Joback Method
cpg	901.04	J/mol×K	833.46	Joback Method

cpg	914.58	J/mol×K	861.80	Joback Method
cpg	927.22	J/mol×K	890.14	Joback Method
cpg	938.95	J/mol×K	918.48	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=U351938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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