

Other names:

2,2,2-trifluoroacetate

3,6,9,12,15,18,21-Heptaoxadocos-1-yl trifluoroacetate

InChI=1S/C17H31F3O9/c1-22-2-3-23-4-5-24-6-7-25-8-9-26-10-11-27-12-13-28-14-15-29

UHWUAIVYARSAHA-UHFFFAOYSA-N

C17H31F3O9

COCCOCCOCCOCCOCCOCCOCCOC(=O)C(F)(F)F

436.42

Property code	Value	Unit	Source
gf	-1458.25	kJ/mol	Joback Method
hf	-2161.63	kJ/mol	Joback Method
hfus	52.71	kJ/mol	Joback Method
hvap	75.72	kJ/mol	Joback Method
log10ws	-0.07		Crippen Method
logp	0.838		Crippen Method
mcvol	304.230	ml/mol	McGowan Method
pc	1082.78	kPa	Joback Method
rinpol	2243.00		NIST Webbook
tb	816.17	K	Joback Method
tc	999.31	K	Joback Method
tf	513.31	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Property code	Value	Unit	Temperature [K]	Source
cpg	975.32	J/mol×K	816.17	Joback Method
cpg	991.83	J/mol×K	846.69	Joback Method
cpg	1007.14	J/mol×K	877.22	Joback Method
cpg	1021.22	J/mol×K	907.74	Joback Method
cpg	1034.06	J/mol×K	938.26	Joback Method
cpg	1045.61	J/mol×K	968.79	Joback Method
cpg	1055.86	J/mol×K	999.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351959&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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