Heptacosyl trifluoroacetate

Other names: Heptacosyl 2,2,2-trifluoroacetate
1-Heptacosanol, trifluoroacetate
Inchi: InChI=1S/C29H55F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: VVPLBTYMPDZWEY-UHFFFAOYSA-N
Formula: C29H55F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 492.74

Physical Properties

Property code	Value	Unit	Source
gf	-622.21	kJ/mol	Joback Method
hf	-1483.77	kJ/mol	Joback Method
hfus	75.48	kJ/mol	Joback Method
hvap	85.56	kJ/mol	Joback Method
log10ws	-11.49		Crippen Method
logp	10.864		Crippen Method
mcvol	432.220	ml/mol	McGowan Method
pc	603.09	kPa	Joback Method
rinpol	2878.20		NIST Webbook
rinpol	2878.20		NIST Webbook
tb	933.79	K	Joback Method
tc	1162.98	K	Joback Method
tf	492.94	K	Joback Method
vc	1.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1502.36	J/mol×K	933.79	Joback Method
cpg	1527.99	J/mol×K	971.99	Joback Method
cpg	1551.87	J/mol×K	1010.19	Joback Method
cpg	1574.13	J/mol×K	1048.38	Joback Method
cpg	1594.87	J/mol×K	1086.58	Joback Method
cpg	1614.23	J/mol×K	1124.78	Joback Method

cpg	1632.33	J/mol×K	1162.98	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=U351758&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