Hexacosyl trifluoroacetate

Other names: Hexacosyl 2,2,2-trifluoroacetate
1-Hexacosanol, trifluoroacetate
Inchi: InChI=1S/C28H53F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: XWYJDXAPLCVABW-UHFFFAOYSA-N
Formula: C28H53F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 478.71

Physical Properties

Property code	Value	Unit	Source
gf	-630.63	kJ/mol	Joback Method
hf	-1463.13	kJ/mol	Joback Method
hfus	72.89	kJ/mol	Joback Method
hvap	83.33	kJ/mol	Joback Method
log10ws	-11.07		Crippen Method
logp	10.474		Crippen Method
mcvol	418.130	ml/mol	McGowan Method
pc	632.57	kPa	Joback Method
rinpol	2780.40		NIST Webbook
tb	910.91	K	Joback Method
tc	1128.73	K	Joback Method
tf	481.67	K	Joback Method
vc	1.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1436.63	J/mol×K	910.91	Joback Method
cpg	1461.19	J/mol×K	947.21	Joback Method
cpg	1484.15	J/mol×K	983.52	Joback Method
cpg	1505.61	J/mol×K	1019.82	Joback Method
cpg	1525.68	J/mol×K	1056.12	Joback Method
cpg	1544.46	J/mol×K	1092.42	Joback Method
cpg	1562.03	J/mol×K	1128.73	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=U351750&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume