Tricosyl trifluoroacetate

Other names: Tricosyl 2,2,2-trifluoroacetate
1-Tricosanol, trifluoroacetate
Inchi: InChI=1S/C25H47F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: JOCVGXYCINXQCU-UHFFFAOYSA-N
Formula: C25H47F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 436.63

Physical Properties

Property code	Value	Unit	Source
gf	-655.89	kJ/mol	Joback Method
hf	-1401.21	kJ/mol	Joback Method
hfus	65.12	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-9.81		Crippen Method
logp	9.304		Crippen Method
mcvol	375.860	ml/mol	McGowan Method
pc	735.22	kPa	Joback Method
rinpol	2489.30		NIST Webbook
tb	842.27	K	Joback Method
tc	1033.43	K	Joback Method
tf	447.86	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.62	J/mol×K	842.27	Joback Method
cpg	1264.48	J/mol×K	874.13	Joback Method
cpg	1285.11	J/mol×K	905.99	Joback Method
cpg	1304.55	J/mol×K	937.85	Joback Method
cpg	1322.87	J/mol×K	969.71	Joback Method
cpg	1340.13	J/mol×K	1001.57	Joback Method
cpg	1356.39	J/mol×K	1033.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351751&Units=SI
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

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