Tetracosyl trifluoroacetate

Other names: Tetracosyl 2,2,2-trifluoroacetate
1-Tetracosanol, trifluoroacetate
Inchi: InChI=1S/C26H49F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: DOXMLSKFEKEMHX-UHFFFAOYSA-N
Formula: C26H49F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 450.66

Physical Properties

Property code	Value	Unit	Source
gf	-647.47	kJ/mol	Joback Method
hf	-1421.85	kJ/mol	Joback Method
hfus	67.71	kJ/mol	Joback Method
hvap	78.88	kJ/mol	Joback Method
log10ws	-10.23		Crippen Method
logp	9.694		Crippen Method
mcvol	389.950	ml/mol	McGowan Method
pc	698.39	kPa	Joback Method
rinpol	2587.70		NIST Webbook
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tb	865.15	K	Joback Method
tc	1064.05	K	Joback Method
tf	459.13	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.72	J/mol×K	865.15	Joback Method
cpg	1329.40	J/mol×K	898.30	Joback Method
cpg	1350.73	J/mol×K	931.45	Joback Method
cpg	1370.79	J/mol×K	964.60	Joback Method
cpg	1389.65	J/mol×K	997.75	Joback Method
cpg	1407.38	J/mol×K	1030.90	Joback Method

cpg	1424.05	J/mol×K	1064.05	Joback Method

Sources

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=U351764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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