Tetracosyl pentafluoropropionate

Other names:	Tetracosyl 2,2,3,3,3-pentafluoropropanoate
	1-Tetracosanol, pentafluoropropionate
Inchi:	InChI=1S/C27H49F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	KOPXDFYIILHNCR-UHFFFAOYSA-N
Formula:	C27H49F5O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	500.67

Physical Properties

Property code	Value	Unit	Source
gf	-1025.83	kJ/mol	Joback Method
hf	-1843.46	kJ/mol	Joback Method
hfus	69.05	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-10.96		Crippen Method
logp	10.329		Crippen Method
mcvol	407.580	ml/mol	McGowan Method
pc	640.60	kPa	Joback Method
rinpol	2580.30		NIST Webbook
rinpol	2580.30		NIST Webbook
tb	883.34	K	Joback Method
tc	1092.29	K	Joback Method
tf	474.00	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1385.41	J/mol×K	883.34	Joback Method
cpg	1408.73	J/mol×K	918.16	Joback Method
cpg	1430.62	J/mol×K	952.99	Joback Method
cpg	1451.19	J/mol×K	987.81	Joback Method
cpg	1470.54	J/mol×K	1022.64	Joback Method
cpg	1488.78	J/mol×K	1057.46	Joback Method

cpg	1506.01	J/mol×K	1092.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351813&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

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

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