Octatriacontyl pentafluoropropionate

Other names:	Octatriacontyl 2,2,3,3,3-pentafluoropropanoate
	1-Octatriacontanol, pentafluoropropionate
Inchi:	InChI=1S/C41H77F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	YWJGNYMMXDJUCM-UHFFFAOYSA-N
Formula:	C41H77F5O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	697.04

Physical Properties

Property code	Value	Unit	Source
gf	-907.95	kJ/mol	Joback Method
hf	-2132.42	kJ/mol	Joback Method
hfus	105.30	kJ/mol	Joback Method
hvap	109.34	kJ/mol	Joback Method
log10ws	-16.82		Crippen Method
logp	15.791		Crippen Method
mcvol	604.840	ml/mol	McGowan Method
pc	356.67	kPa	Joback Method
rinpol	3938.40		NIST Webbook
rinpol	3938.40		NIST Webbook
tb	1203.66	K	Joback Method
tc	1741.75	K	Joback Method
tf	631.78	K	Joback Method
vc	2.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2330.87	J/mol×K	1203.66	Joback Method
cpg	2385.10	J/mol×K	1293.34	Joback Method
cpg	2435.56	J/mol×K	1383.02	Joback Method
cpg	2484.79	J/mol×K	1472.70	Joback Method
cpg	2535.32	J/mol×K	1562.38	Joback Method
cpg	2589.67	J/mol×K	1652.07	Joback Method

cpg	2650.38	J/mol×K	1741.75	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=U351891&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