Pentafluoropropionic acid, pentadecyl ester

Other names: Pentadecyl pentafluoropropionate
Inchi: InChI=1S/C18H31F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-25-16(24)17(19,20)18(21
InchiKey: SOIQTDZYLNEIHG-UHFFFAOYSA-N
Formula: C18H31F5O2
SMILES: CCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 374.43
CAS: 959092-08-1

Physical Properties

Property code	Value	Unit	Source
gf	-1101.61	kJ/mol	Joback Method
hf	-1657.70	kJ/mol	Joback Method
hfus	45.73	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	6.818		Crippen Method
mcvol	280.770	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1733.20		NIST Webbook
tb	677.42	K	Joback Method
tc	835.92	K	Joback Method
tf	372.57	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.94	J/mol×K	677.42	Joback Method
cpg	850.11	J/mol×K	703.84	Joback Method
cpg	866.45	J/mol×K	730.25	Joback Method
cpg	881.99	J/mol×K	756.67	Joback Method
cpg	896.77	J/mol×K	783.09	Joback Method
cpg	910.82	J/mol×K	809.50	Joback Method

cpg	924.18	J/mol×K	835.92	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=C959092081&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