

Pentafluoropropionic acid, octadecyl ester

Other names:	Octadecyl pentafluoropropionate
Inchi:	InChI=1S/C21H37F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-28-19(27)20(22)
InchiKey:	KNCMVQBRQJKYNM-UHFFFAOYSA-N
Formula:	C21H37F5O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	416.51
CAS:	959261-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-1076.35	kJ/mol	Joback Method
hf	-1719.62	kJ/mol	Joback Method
hfus	53.51	kJ/mol	Joback Method
hvap	64.82	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	7.989		Crippen Method
mcvol	323.040	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	2054.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	2008.00		NIST Webbook
ripol	2097.00		NIST Webbook
tb	746.06	K	Joback Method
tc	914.00	K	Joback Method
tf	406.38	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.73	J/molxK	746.06	Joback Method
cpg	1028.45	J/molxK	774.05	Joback Method

cpg	1046.22	J/mol×K	802.04	Joback Method
cpg	1063.07	J/mol×K	830.03	Joback Method
cpg	1079.07	J/mol×K	858.02	Joback Method
cpg	1094.24	J/mol×K	886.01	Joback Method
cpg	1108.65	J/mol×K	914.00	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=C959261257&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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