Pentafluoropropionic acid, heptadecyl ester

Other names: Heptadecyl pentafluoropropionate
Inchi: InChI=1S/C20H35F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-27-18(26)19(21,22
InchiKey: YUZPMKBRUISFHZ-UHFFFAOYSA-N
Formula: C20H35F5O2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 402.48
CAS: 959218-78-1

Physical Properties

Property code	Value	Unit	Source
gf	-1084.77	kJ/mol	Joback Method
hf	-1698.98	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.599		Crippen Method
mcvol	308.950	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	1912.70		NIST Webbook
rinpol	1909.00		NIST Webbook
tb	723.18	K	Joback Method
tc	887.32	K	Joback Method
tf	395.11	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.84	J/mol×K	723.18	Joback Method
cpg	968.01	J/mol×K	750.54	Joback Method
cpg	985.27	J/mol×K	777.89	Joback Method
cpg	1001.67	J/mol×K	805.25	Joback Method
cpg	1017.24	J/mol×K	832.61	Joback Method
cpg	1032.02	J/mol×K	859.96	Joback Method

cpg	1046.06	J/mol×K	887.32	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=C959218781&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