Heptafluorobutyric acid, pentadecyl ester

Other names: Pentadecyl heptafluorobutyrate
Inchi: InChI=1S/C19H31F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-28-16(27)17(20,21)18(22
InchiKey: LSNYOOKRVAXMSQ-UHFFFAOYSA-N
Formula: C19H31F7O2
SMILES: CCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 424.44
CAS: 959261-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-1479.97	kJ/mol	Joback Method
hf	-2079.31	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	57.44	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	7.454		Crippen Method
mcvol	298.400	ml/mol	McGowan Method
pc	944.42	kPa	Joback Method
rinpol	1764.40		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	695.61	K	Joback Method
tc	854.36	K	Joback Method
tf	387.44	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.32	J/mol×K	695.61	Joback Method
cpg	925.47	J/mol×K	722.07	Joback Method
cpg	941.75	J/mol×K	748.53	Joback Method
cpg	957.19	J/mol×K	774.99	Joback Method
cpg	971.83	J/mol×K	801.45	Joback Method
cpg	985.73	J/mol×K	827.90	Joback Method

cpg	998.92	J/mol×K	854.36	Joback Method

Sources

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=C959261235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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