Pentafluoropropionic acid, tridecyl ester

Other names: Tridecyl pentafluoropropionate
Inchi: InChI=1S/C16H27F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-23-14(22)15(17,18)16(19,20)21/
InchiKey: WGTROCTZHUYVJI-UHFFFAOYSA-N
Formula: C16H27F5O2
SMILES: CCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 346.38
CAS: 959261-22-4

Physical Properties

Property code	Value	Unit	Source
gf	-1118.45	kJ/mol	Joback Method
hf	-1616.42	kJ/mol	Joback Method
hfus	40.55	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	6.038		Crippen Method
mcvol	252.590	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1534.50		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1534.50		NIST Webbook
tb	631.66	K	Joback Method
tc	786.72	K	Joback Method
tf	350.03	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.36	J/mol×K	631.66	Joback Method
cpg	736.59	J/mol×K	657.50	Joback Method
cpg	752.06	J/mol×K	683.35	Joback Method
cpg	766.79	J/mol×K	709.19	Joback Method

cpg	780.81	J/mol×K	735.03	Joback Method
cpg	794.15	J/mol×K	760.87	Joback Method
cpg	806.84	J/mol×K	786.72	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=C959261224&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