Pentafluoropropionic acid, tetradecyl ester

Inchi: InChI=1S/C17H29F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-24-15(23)16(18,19)17(20,21)
InchiKey: JOQINMMRCSNJTD-UHFFFAOYSA-N
Formula: C17H29F5O2
SMILES: CCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 360.40
CAS: 6222-06-6

Physical Properties

Property code	Value	Unit	Source
gf	-1110.03	kJ/mol	Joback Method
hf	-1637.06	kJ/mol	Joback Method
hfus	43.15	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.428		Crippen Method
mcvol	266.680	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	1639.10		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1627.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1701.00		NIST Webbook
tb	654.54	K	Joback Method
tc	811.07	K	Joback Method
tf	361.30	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.07	J/mol×K	654.54	Joback Method
cpg	792.77	J/mol×K	680.63	Joback Method
cpg	808.67	J/mol×K	706.72	Joback Method
cpg	823.81	J/mol×K	732.81	Joback Method

cpg	838.21	J/mol×K	758.90	Joback Method
cpg	851.90	J/mol×K	784.98	Joback Method
cpg	864.93	J/mol×K	811.07	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=C6222066&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume