

Peroxytridecanoic acid

Inchi:	InChI=1S/C13H26O3/c1-2-3-4-5-6-7-8-9-10-11-12-13(14)16-15/h15H,2-12H2,1H3
InchiKey:	LOYQGUVUOVODCG-UHFFFAOYSA-N
Formula:	C13H26O3
SMILES:	CCCCCCCCCCCC(=O)OO
Mol. weight [g/mol]:	230.34
CAS:	40915-96-6

Physical Properties

Property code	Value	Unit	Source
gf	-312.16	kJ/mol	Joback Method
hf	-708.68	kJ/mol	Joback Method
hfus	36.30	kJ/mol	Joback Method
hsub	143.00 ± 5.00	kJ/mol	NIST Webbook
hvap	70.37	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.314		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
tb	665.31	K	Joback Method
tc	832.17	K	Joback Method
tf	369.25	K	Joback Method
vc	0.806	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.17	J/mol×K	665.31	Joback Method
cpg	597.40	J/mol×K	693.12	Joback Method
cpg	611.03	J/mol×K	720.93	Joback Method
cpg	624.05	J/mol×K	748.74	Joback Method
cpg	636.47	J/mol×K	776.55	Joback Method
cpg	648.32	J/mol×K	804.36	Joback Method
cpg	659.59	J/mol×K	832.17	Joback Method
dvisc	0.0035060	Paxs	369.25	Joback Method

dvisc	0.0011030	Paxs	418.59	Joback Method
dvisc	0.0004429	Paxs	467.94	Joback Method
dvisc	0.0002116	Paxs	517.28	Joback Method
dvisc	0.0001150	Paxs	566.62	Joback Method
dvisc	0.0000689	Paxs	615.97	Joback Method
dvisc	0.0000446	Paxs	665.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C40915966&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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