Octacosane-7,9-dione

Inchi: InChI=1S/C28H54O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-23-25-28(30)26-
InchiKey: IWCFDKOWVIQRIU-UHFFFAOYSA-N
Formula: C28H54O2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)CC(=O)CCCCCC
Mol. weight [g/mol]: 422.73

Physical Properties

Property code	Value	Unit	Source
gf	-72.96	kJ/mol	Joback Method
hf	-846.41	kJ/mol	Joback Method
hfus	71.47	kJ/mol	Joback Method
hvap	91.41	kJ/mol	Joback Method
log10ws	-10.10		Crippen Method
logp	9.527		Crippen Method
mcvol	408.520	ml/mol	McGowan Method
pc	699.87	kPa	Joback Method
rinpol	3092.30		NIST Webbook
rinpol	3092.30		NIST Webbook
tb	947.78	K	Joback Method
tc	1168.46	K	Joback Method
tf	505.18	K	Joback Method
vc	1.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.27	J/mol×K	947.78	Joback Method
cpg	1432.59	J/mol×K	984.56	Joback Method
cpg	1454.38	J/mol×K	1021.34	Joback Method
cpg	1474.73	J/mol×K	1058.12	Joback Method
cpg	1493.74	J/mol×K	1094.90	Joback Method
cpg	1511.50	J/mol×K	1131.68	Joback Method
cpg	1528.09	J/mol×K	1168.46	Joback Method
dvisc	0.0007023	Pa×s	505.18	Joback Method

dvisc	0.0002950	Pa×s	578.95	Joback Method
dvisc	0.0001507	Pa×s	652.71	Joback Method
dvisc	0.0000883	Pa×s	726.48	Joback Method
dvisc	0.0000571	Pa×s	800.25	Joback Method
dvisc	0.0000397	Pa×s	874.01	Joback Method
dvisc	0.0000292	Pa×s	947.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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