7,9-Docosanedione

Other names: Docosane-7,9-dione
Inchi: InChI=1S/C22H42O2/c1-3-5-7-9-10-11-12-13-14-15-17-19-22(24)20-21(23)18-16-8-6-4-2
InchiKey: GDFKEQLEKXGCJB-UHFFFAOYSA-N
Formula: C22H42O2
SMILES: CCCCCCCCCCCCCC(=O)CC(=O)CCCCCC
Mol. weight [g/mol]: 338.57
CAS: 52262-76-7

Physical Properties

Property code	Value	Unit	Source
gf	-123.48	kJ/mol	Joback Method
hf	-722.57	kJ/mol	Joback Method
hfus	55.93	kJ/mol	Joback Method
hvap	78.06	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	7.186		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	974.13	kPa	Joback Method
rinpol	2479.80		NIST Webbook
tb	810.50	K	Joback Method
tc	994.05	K	Joback Method
tf	437.56	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.09	J/mol×K	810.50	Joback Method
cpg	1046.61	J/mol×K	841.09	Joback Method
cpg	1065.10	J/mol×K	871.68	Joback Method
cpg	1082.60	J/mol×K	902.27	Joback Method
cpg	1099.16	J/mol×K	932.86	Joback Method
cpg	1114.81	J/mol×K	963.45	Joback Method
cpg	1129.59	J/mol×K	994.05	Joback Method

dvisc	0.0014616	Pa×s	437.56	Joback Method
dvisc	0.0006456	Pa×s	499.72	Joback Method
dvisc	0.0003417	Pa×s	561.87	Joback Method
dvisc	0.0002053	Pa×s	624.03	Joback Method
dvisc	0.0001352	Pa×s	686.19	Joback Method
dvisc	0.0000955	Pa×s	748.34	Joback Method
dvisc	0.0000711	Pa×s	810.50	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52262767&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
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