

Docosane-6,8-dione

Inchi:	InChI=1S/C22H42O2/c1-3-5-7-8-9-10-11-12-13-14-15-17-19-22(24)20-21(23)18-16-6-4-2
InchiKey:	JFNKGJXCTSFELO-UHFFFAOYSA-N
Formula:	C22H42O2
SMILES:	CCCCCCCCCCCCCCCC(=O)CC(=O)CCCC
Mol. weight [g/mol]:	338.57

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
mvol	323.980	ml/mol	McGowan Method
pc	974.13	kPa	Joback Method
rinpol	2482.20		NIST Webbook
rinpol	2482.20		NIST Webbook
tb	810.50	K	Joback Method
tc	994.05	K	Joback Method
tf	437.56	K	Joback Method
vc	1.280	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.09	J/molxK	810.50	Joback Method
cpg	1046.61	J/molxK	841.09	Joback Method
cpg	1065.10	J/molxK	871.68	Joback Method
cpg	1082.60	J/molxK	902.27	Joback Method
cpg	1099.16	J/molxK	932.86	Joback Method
cpg	1114.81	J/molxK	963.45	Joback Method
cpg	1129.59	J/molxK	994.05	Joback Method
dvisc	0.0014616	Paxs	437.56	Joback Method

dvisc	0.0006456	Paxs	499.72	Joback Method
dvisc	0.0003417	Paxs	561.87	Joback Method
dvisc	0.0002053	Paxs	624.03	Joback Method
dvisc	0.0001352	Paxs	686.19	Joback Method
dvisc	0.0000955	Paxs	748.34	Joback Method
dvisc	0.0000711	Paxs	810.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413381&Units=SI
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

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

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