

Pentacosane-4,6-dione

Inchi:	InChI=1S/C25H48O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-25(27)23-24
InchiKey:	OHQHRHJGILPHCW-UHFFFAOYSA-N
Formula:	C25H48O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)CC(=O)CCC
Mol. weight [g/mol]:	380.65
CAS:	289681-94-3

Physical Properties

Property code	Value	Unit	Source
gf	-98.22	kJ/mol	Joback Method
hf	-784.49	kJ/mol	Joback Method
hfus	63.70	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	8.357		Crippen Method
mcvol	366.250	ml/mol	McGowan Method
pc	820.07	kPa	Joback Method
rinpol	2787.70		NIST Webbook
rinpol	2787.70		NIST Webbook
tb	879.14	K	Joback Method
tc	1076.77	K	Joback Method
tf	471.37	K	Joback Method
vc	1.448	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.41	J/mol×K	879.14	Joback Method
cpg	1236.55	J/mol×K	912.08	Joback Method
cpg	1256.47	J/mol×K	945.02	Joback Method
cpg	1275.22	J/mol×K	977.96	Joback Method
cpg	1292.86	J/mol×K	1010.89	Joback Method
cpg	1309.44	J/mol×K	1043.83	Joback Method
cpg	1325.03	J/mol×K	1076.77	Joback Method

dvisc	0.0010282	Paxs	471.37	Joback Method
dvisc	0.0004421	Paxs	539.33	Joback Method
dvisc	0.0002297	Paxs	607.29	Joback Method
dvisc	0.0001361	Paxs	675.25	Joback Method
dvisc	0.0000888	Paxs	743.22	Joback Method
dvisc	0.0000622	Paxs	811.18	Joback Method
dvisc	0.0000460	Paxs	879.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C289681943&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

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