

Pentacosane-6,8-dione

Inchi:	InChI=1S/C25H48O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-22-25(27)23-24(26)2
InchiKey:	ZQDADPUQAZWEGX-UHFFFAOYSA-N
Formula:	C25H48O2
SMILES:	CCCCCCCCCCCCCCCCC(=O)CC(=O)CCCC
Mol. weight [g/mol]:	380.65
CAS:	289681-95-4

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
mvol	366.250	ml/mol	McGowan Method
pc	820.07	kPa	Joback Method
rinpol	2780.90		NIST Webbook
rinpol	2780.90		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/molxK	879.14	Joback Method
cpg	1236.55	J/molxK	912.08	Joback Method
cpg	1256.47	J/molxK	945.02	Joback Method
cpg	1275.22	J/molxK	977.96	Joback Method
cpg	1292.86	J/molxK	1010.89	Joback Method
cpg	1309.44	J/molxK	1043.83	Joback Method
cpg	1325.03	J/molxK	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

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=C289681954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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