

Heptacosane-4,6-dione

Inchi:	InChI=1S/C27H52O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-27(29
InchiKey:	PWIHAABDKZGMJA-UHFFFAOYSA-N
Formula:	C27H52O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)CC(=O)CCC
Mol. weight [g/mol]:	408.70

Physical Properties

Property code	Value	Unit	Source
gf	-81.38	kJ/mol	Joback Method
hf	-825.77	kJ/mol	Joback Method
hfus	68.88	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-9.68		Crippen Method
logp	9.137		Crippen Method
mcvol	394.430	ml/mol	McGowan Method
pc	736.82	kPa	Joback Method
rinpol	2996.30		NIST Webbook
rinpol	2996.30		NIST Webbook
tb	924.90	K	Joback Method
tc	1136.76	K	Joback Method
tf	493.91	K	Joback Method
vc	1.560	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.12	J/molxK	924.90	Joback Method
cpg	1366.64	J/molxK	960.21	Joback Method
cpg	1387.74	J/molxK	995.52	Joback Method
cpg	1407.51	J/molxK	1030.83	Joback Method
cpg	1426.03	J/molxK	1066.14	Joback Method
cpg	1443.36	J/molxK	1101.45	Joback Method
cpg	1459.59	J/molxK	1136.76	Joback Method
dvisc	0.0007997	Paxs	493.91	Joback Method

dvisc	0.0003384	Paxs	565.74	Joback Method
dvisc	0.0001739	Paxs	637.57	Joback Method
dvisc	0.0001022	Paxs	709.40	Joback Method
dvisc	0.0000662	Paxs	781.24	Joback Method
dvisc	0.0000462	Paxs	853.07	Joback Method
dvisc	0.0000341	Paxs	924.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413396&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
mccvol:	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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