Heptadecane-2,4-dione

Other names: 2,4-Heptadecadione
Inchi: InChI=1S/C17H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-17(19)15-16(2)18/h3-15H2,1-2H3
InchiKey: VZRNDOSIHXJXCH-UHFFFAOYSA-N
Formula: C17H32O2
SMILES: CCCCCCCCCCCCCC(=O)CC(C)=O
Mol. weight [g/mol]: 268.43
CAS: 64042-18-8

Physical Properties

Property code	Value	Unit	Source
gf	-165.58	kJ/mol	Joback Method
hf	-619.37	kJ/mol	Joback Method
hfus	42.98	kJ/mol	Joback Method
hvap	66.93	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.236		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	696.10	K	Joback Method
tc	870.97	K	Joback Method
tf	381.21	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.94	J/mol×K	696.10	Joback Method
cpg	809.00	J/mol×K	841.83	Joback Method
cpg	794.74	J/mol×K	812.68	Joback Method
cpg	779.73	J/mol×K	783.54	Joback Method
cpg	763.95	J/mol×K	754.39	Joback Method
cpg	747.36	J/mol×K	725.25	Joback Method

cpg	822.54	J/mol×K	870.97	Joback Method
dvisc	0.0001389	Pa×s	696.10	Joback Method
dvisc	0.0001841	Pa×s	643.62	Joback Method
dvisc	0.0002565	Pa×s	591.14	Joback Method
dvisc	0.0003812	Pa×s	538.65	Joback Method
dvisc	0.0006170	Pa×s	486.17	Joback Method
dvisc	0.0011224	Pa×s	433.69	Joback Method
dvisc	0.0024071	Pa×s	381.21	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=C64042188&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

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