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]: 268.44

Physical Properties

Property code	Value	Unit	Source
af	0.8319		Cheméo Relay (1.0)
gf	-165.58	kJ/mol	Joback Method
hf	-647.76	kJ/mol	Cheméo Relay (1.0)
hfus	42.98	kJ/mol	Joback Method
hvap	82.55	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-5.59		Cheméo Relay (1.0)
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	582.48	K	Cheméo Relay (1.0)
tc	775.11	K	Cheméo Relay (1.0)
tf	339.32	K	Cheméo Relay (1.0)
vc	0.961	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	809.00	J/mol×K	841.83	Joback Method
cpg	822.54	J/mol×K	870.97	Joback Method
dvisc	0.0024071	Pa×s	381.21	Joback Method
dvisc	0.0011224	Pa×s	433.69	Joback Method
dvisc	0.0006170	Pa×s	486.17	Joback Method
dvisc	0.0003812	Pa×s	538.65	Joback Method
dvisc	0.0002565	Pa×s	591.14	Joback Method
dvisc	0.0001841	Pa×s	643.62	Joback Method
dvisc	0.0001389	Pa×s	696.10	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64042188&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
ie: Ionization energy
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