2,4-Dimethyl-heptane-3,5-dione

Other names: 2,4-Dimethylheptan-3,5-dione
Inchi: InChI=1S/C9H16O2/c1-5-8(10)7(4)9(11)6(2)3/h6-7H,5H2,1-4H3
InchiKey: QLURKUIFEGCQQS-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CCC(=O)C(C)C(=O)C(C)C
Mol. weight [g/mol]: 156.22
CAS: 37484-68-7

Physical Properties

Property code	Value	Unit	Source
gf	-237.82	kJ/mol	Joback Method
hf	-464.81	kJ/mol	Joback Method
hfus	15.22	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.827		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1068.00		NIST Webbook
rinpol	1111.80		NIST Webbook
rinpol	1111.80		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1068.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1523.00		NIST Webbook
tb	512.18	K	Joback Method
tc	703.77	K	Joback Method
tf	261.05	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.58	J/mol×K	512.18	Joback Method
cpg	332.99	J/mol×K	544.11	Joback Method
cpg	345.76	J/mol×K	576.04	Joback Method
cpg	357.91	J/mol×K	607.98	Joback Method
cpg	369.47	J/mol×K	639.91	Joback Method
cpg	380.44	J/mol×K	671.84	Joback Method
cpg	390.83	J/mol×K	703.77	Joback Method
dvisc	0.0071523	Pa×s	261.05	Joback Method
dvisc	0.0028688	Pa×s	302.91	Joback Method
dvisc	0.0014364	Pa×s	344.76	Joback Method
dvisc	0.0008354	Pa×s	386.62	Joback Method
dvisc	0.0005402	Pa×s	428.47	Joback Method
dvisc	0.0003774	Pa×s	470.33	Joback Method
dvisc	0.0002796	Pa×s	512.18	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=C37484687&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume