4-Methylheptane-3,5-dione

Inchi: InChI=1S/C8H14O2/c1-4-7(9)6(3)8(10)5-2/h6H,4-5H2,1-3H3
InchiKey: FIJLPSJMPXGRJL-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CCC(=O)C(C)C(=O)CC
Mol. weight [g/mol]: 142.20
CAS: 1187-04-8

Physical Properties

Property code	Value	Unit	Source
gf	-243.80	kJ/mol	Joback Method
hf	-438.89	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	46.51	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.581		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1055.90		NIST Webbook
rinpol	1055.90		NIST Webbook
tb	489.74	K	Joback Method
tc	679.53	K	Joback Method
tf	264.78	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.42	J/mol×K	489.74	Joback Method
cpg	287.52	J/mol×K	521.37	Joback Method
cpg	299.07	J/mol×K	553.00	Joback Method
cpg	310.09	J/mol×K	584.63	Joback Method
cpg	320.57	J/mol×K	616.27	Joback Method
cpg	330.55	J/mol×K	647.90	Joback Method
cpg	340.02	J/mol×K	679.53	Joback Method

dvisc	0.0050267	Pa×s	264.78	Joback Method
dvisc	0.0023823	Pa×s	302.27	Joback Method
dvisc	0.0013314	Pa×s	339.77	Joback Method
dvisc	0.0008352	Pa×s	377.26	Joback Method
dvisc	0.0005701	Pa×s	414.75	Joback Method
dvisc	0.0004145	Pa×s	452.25	Joback Method
dvisc	0.0003165	Pa×s	489.74	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=C1187048&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