(R,S)-5-Ethyl-6-methyl-3E-hepten-2-one

Inchi: InChI=1S/C10H18O/c1-5-10(8(2)3)7-6-9(4)11/h6-8,10H,5H2,1-4H3/b7-6+
InchiKey: BCYUENXUQILNAA-VOTSOKGWSA-N
Formula: C10H18O
SMILES: CCC(C=CC(C)=O)C(C)C
Mol. weight [g/mol]: 154.25
CAS: 57283-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-20.26	kJ/mol	Joback Method
hf	-255.65	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	43.78	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.814		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1143.90		NIST Webbook
rinpol	1143.90		NIST Webbook
rinpol	1124.30		NIST Webbook
tb	485.35	K	Joback Method
tc	673.78	K	Joback Method
tf	217.31	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.63	J/mol×K	485.35	Joback Method
cpg	393.12	J/mol×K	642.38	Joback Method
cpg	380.96	J/mol×K	610.97	Joback Method
cpg	368.16	J/mol×K	579.57	Joback Method
cpg	354.69	J/mol×K	548.16	Joback Method
cpg	340.52	J/mol×K	516.76	Joback Method

cpg	404.66	J/mol×K	673.78	Joback Method
dvisc	0.0002025	Pa×s	485.35	Joback Method
dvisc	0.0002800	Pa×s	440.68	Joback Method
dvisc	0.0004163	Pa×s	396.00	Joback Method
dvisc	0.0006849	Pa×s	351.33	Joback Method
dvisc	0.0013024	Pa×s	306.66	Joback Method
dvisc	0.0030838	Pa×s	261.98	Joback Method
dvisc	0.0104075	Pa×s	217.31	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57283791&Units=SI
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

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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