2,4-heptadien-1-ol

Inchi: InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h3-6,8H,2,7H2,1H3/b4-3+,6-5+
InchiKey: MDRZSADXFOPYOC-VNKDHWASSA-N
Formula: C7H12O
SMILES: CCC=CC=CCO
Mol. weight [g/mol]: 112.17
CAS: 62488-55-5

Physical Properties

Property code	Value	Unit	Source
gf	31.68	kJ/mol	Joback Method
hf	-105.60	kJ/mol	Joback Method
hfus	18.38	kJ/mol	Joback Method
hvap	47.77	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.501		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1696.00		NIST Webbook
tb	460.06	K	Joback Method
tc	635.58	K	Joback Method
tf	219.31	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.93	J/mol×K	460.06	Joback Method
cpg	224.74	J/mol×K	489.31	Joback Method
cpg	234.05	J/mol×K	518.57	Joback Method
cpg	242.87	J/mol×K	547.82	Joback Method
cpg	251.25	J/mol×K	577.07	Joback Method

cpg	259.20	J/mol×K	606.33	Joback Method
cpg	266.74	J/mol×K	635.58	Joback Method
dvisc	0.0758665	Pa×s	219.31	Joback Method
dvisc	0.0117756	Pa×s	259.44	Joback Method
dvisc	0.0030106	Pa×s	299.56	Joback Method
dvisc	0.0010624	Pa×s	339.69	Joback Method
dvisc	0.0004672	Pa×s	379.81	Joback Method
dvisc	0.0002404	Pa×s	419.94	Joback Method
dvisc	0.0001389	Pa×s	460.06	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=C62488555&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