

2,4-Heptadien-1-ol, (E,E)-

Other names:	(E,E)-2,4-Heptadien-1-ol 2,4-Heptadien-1-ol (2E,4E)-hepta-2,4-dien-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:	33467-79-7

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
ripol	1682.00		NIST Webbook
ripol	1682.00		NIST Webbook
tb	460.06	K	Joback Method
tc	635.58	K	Joback Method
tf	219.31	K	Joback Method
vc	0.406	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.93	J/mol×K	460.06	Joback Method
cpg	259.20	J/mol×K	606.33	Joback Method
cpg	251.25	J/mol×K	577.07	Joback Method
cpg	242.87	J/mol×K	547.82	Joback Method

cpg	234.05	J/mol×K	518.57	Joback Method
cpg	224.74	J/mol×K	489.31	Joback Method
cpg	266.74	J/mol×K	635.58	Joback Method
dvisc	0.0001389	Paxs	460.06	Joback Method
dvisc	0.0002404	Paxs	419.94	Joback Method
dvisc	0.0004672	Paxs	379.81	Joback Method
dvisc	0.0010624	Paxs	339.69	Joback Method
dvisc	0.0030106	Paxs	299.56	Joback Method
dvisc	0.0117756	Paxs	259.44	Joback Method
dvisc	0.0758665	Paxs	219.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C33467797&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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