

1,3-Dioxepane, 2-heptyl-

Other names:	2-Heptyl-1,3-dioxepane
Inchi:	InChI=1S/C12H24O2/c1-2-3-4-5-6-9-12-13-10-7-8-11-14-12/h12H,2-11H2,1H3
InchiKey:	JPISZFLCOGWKHT-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCCC1OCCCCO1
Mol. weight [g/mol]:	200.32
CAS:	61732-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-109.73	kJ/mol	Joback Method
hf	-506.85	kJ/mol	Joback Method
hfus	32.53	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.500		Crippen Method
mcvol	180.820	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	551.68	K	Joback Method
tc	748.95	K	Joback Method
tf	282.00	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.13	J/mol×K	748.95	Joback Method
cpg	559.68	J/mol×K	716.07	Joback Method
cpg	543.29	J/mol×K	683.19	Joback Method
cpg	525.94	J/mol×K	650.32	Joback Method
cpg	507.61	J/mol×K	617.44	Joback Method
cpg	488.28	J/mol×K	584.56	Joback Method
cpg	467.93	J/mol×K	551.68	Joback Method
dvisc	0.0086681	Pa×s	282.00	Joback Method

dvisc	0.0001811	Pa×s	551.68	Joback Method
dvisc	0.0002592	Pa×s	506.73	Joback Method
dvisc	0.0003979	Pa×s	461.79	Joback Method
dvisc	0.0006701	Pa×s	416.84	Joback Method
dvisc	0.0012798	Pa×s	371.89	Joback Method
dvisc	0.0029203	Pa×s	326.95	Joback Method
hvapt	70.30	kJ/mol	350.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61732921&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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