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: CCCCCCCC1OCCCCO1
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
af	0.5250		Cheméo Relay (1.0)
gf	-109.73	kJ/mol	Joback Method
hf	-528.09	kJ/mol	Cheméo Relay (1.0)
hfus	32.53	kJ/mol	Joback Method
hvap	64.47	kJ/mol	Cheméo Relay (1.0)
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-3.29		Cheméo Relay (1.0)
logp	3.500		Crippen Method
mcvol	180.820	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	527.68	K	Cheméo Relay (1.0)
tc	714.28	K	Cheméo Relay (1.0)
tf	253.64	K	Cheméo Relay (1.0)
vc	0.687	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.93	J/mol×K	551.68	Joback Method
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

dvisc	0.0006701	Pa×s	416.84	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	0.0086681	Pa×s	282.00	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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61732921&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
ie: Ionization energy
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