1,3-DIOXOLANE, 2-HEPTYL-

Other names: 2-heptyl-1,3-dioxolane
Inchi: InChI=1S/C10H20O2/c1-2-3-4-5-6-7-10-11-8-9-12-10/h10H,2-9H2,1H3
InchiKey: LWJBQKKNODYJEI-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCCCCCCC1OCCO1
Mol. weight [g/mol]: 172.27

Physical Properties

Property code	Value	Unit	Source
af	0.5151		Cheméo Relay (1.0)
gf	-102.37	kJ/mol	Joback Method
hf	-470.75	kJ/mol	Cheméo Relay (1.0)
hfus	31.55	kJ/mol	Joback Method
hvap	58.86	kJ/mol	Cheméo Relay (1.0)
ie	9.69	eV	Cheméo Relay (1.0)
log10ws	-3.08		Cheméo Relay (1.0)
logp	2.720		Crippen Method
mcvol	152.640	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	485.72	K	Cheméo Relay (1.0)
tc	672.25	K	Cheméo Relay (1.0)
tf	243.99	K	Cheméo Relay (1.0)
vc	0.601	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.50	J/mol×K	654.70	Joback Method
cpg	458.83	J/mol×K	686.16	Joback Method
cpg	384.72	J/mol×K	528.84	Joback Method
cpg	401.09	J/mol×K	560.31	Joback Method
cpg	416.65	J/mol×K	591.77	Joback Method
cpg	431.45	J/mol×K	623.23	Joback Method
cpg	367.54	J/mol×K	497.38	Joback Method

dvisc	0.0014886	Pa×s	343.46	Joback Method
dvisc	0.0026959	Pa×s	304.98	Joback Method
dvisc	0.0057959	Pa×s	266.50	Joback Method
dvisc	0.0009265	Pa×s	381.94	Joback Method
dvisc	0.0006289	Pa×s	420.42	Joback Method
dvisc	0.0004556	Pa×s	458.90	Joback Method
dvisc	0.0003469	Pa×s	497.38	Joback Method
hvapt	62.00	kJ/mol	385.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4359573&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

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

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