

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]:	172.26
CAS:	4359-57-3

Physical Properties

Property code	Value	Unit	Source
gf	-102.37	kJ/mol	Joback Method
hf	-453.25	kJ/mol	Joback Method
hfus	31.55	kJ/mol	Joback Method
hvap	47.13	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.720		Crippen Method
mcvol	152.640	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	497.38	K	Joback Method
tc	686.16	K	Joback Method
tf	266.50	K	Joback Method
vc	0.579	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.54	J/mol×K	497.38	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	445.50	J/mol×K	654.70	Joback Method
cpg	458.83	J/mol×K	686.16	Joback Method
dvisc	0.0057959	Paxs	266.50	Joback Method

dvisc	0.0026959	Paxs	304.98	Joback Method
dvisc	0.0014886	Paxs	343.46	Joback Method
dvisc	0.0009265	Paxs	381.94	Joback Method
dvisc	0.0006289	Paxs	420.42	Joback Method
dvisc	0.0004556	Paxs	458.90	Joback Method
dvisc	0.0003469	Paxs	497.38	Joback Method
hvapt	62.00	kJ/mol	385.50	NIST Webbook

Sources

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=C4359573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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