

Decanol

Inchi: InChI=1S/C10H22O/c1-2-3-4-5-6-7-8-9-10-11/h11H,2-10H2,1H3
InchiKey: MWKFXSUHUHTGQN-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCCCCCCCO
Mol. weight [g/mol]: 158.28
CAS: 36729-58-5

Physical Properties

Property code	Value	Unit	Source
gf	-103.50	kJ/mol	Joback Method
hf	-401.96	kJ/mol	Joback Method
hfus	25.74	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.119		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1270.00		NIST Webbook
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ripol	1765.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1784.90		NIST Webbook
ripol	1770.90		NIST Webbook
ripol	1763.10		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1782.40		NIST Webbook
ripol	1720.00		NIST Webbook
tb	520.38	K	Joback Method
tc	678.87	K	Joback Method

tf	263.28	K	Joback Method
vc	0.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.60	J/mol×K	520.38	Joback Method
cpg	441.87	J/mol×K	652.45	Joback Method
cpg	430.56	J/mol×K	626.04	Joback Method
cpg	418.80	J/mol×K	599.62	Joback Method
cpg	406.56	J/mol×K	573.21	Joback Method
cpg	393.83	J/mol×K	546.79	Joback Method
cpg	452.73	J/mol×K	678.87	Joback Method
dvisc	0.0001241	Paxs	520.38	Joback Method
dvisc	0.0002072	Paxs	477.53	Joback Method
dvisc	0.0003827	Paxs	434.68	Joback Method
dvisc	0.0008083	Paxs	391.83	Joback Method
dvisc	0.0020510	Paxs	348.98	Joback Method
dvisc	0.0067547	Paxs	306.13	Joback Method
dvisc	0.0327895	Paxs	263.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36729585&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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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