2-DODECANOL, 2-METHYL-

Other names: 2-Methyl-2-dodecanol
Inchi: InChI=1S/C13H28O/c1-4-5-6-7-8-9-10-11-12-13(2,3)14/h14H,4-12H2,1-3H3
InchiKey: YVVFTTGYNOVKSI-UHFFFAOYSA-N
Formula: C13H28O
SMILES: CCCCCCCCCCC(C)(C)O
Mol. weight [g/mol]: 200.37

Physical Properties

Property code	Value	Unit	Source
af	0.8184		Cheméo Relay (1.0)
gf	-75.40	kJ/mol	Joback Method
hf	-505.93	kJ/mol	Cheméo Relay (1.0)
hfus	26.10	kJ/mol	Joback Method
hvap	84.35	kJ/mol	Cheméo Relay (1.0)
ie	9.79	eV	Cheméo Relay (1.0)
log10ws	-4.69		Cheméo Relay (1.0)
logp	4.288		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
tb	526.49	K	Cheméo Relay (1.0)
tc	697.34	K	Cheméo Relay (1.0)
tf	296.74	K	Cheméo Relay (1.0)
vc	0.777	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.58	J/mol×K	585.79	Joback Method
cpg	548.46	J/mol×K	613.17	Joback Method
cpg	563.62	J/mol×K	640.55	Joback Method
cpg	578.11	J/mol×K	667.93	Joback Method
cpg	591.95	J/mol×K	695.32	Joback Method
cpg	605.16	J/mol×K	722.70	Joback Method
cpg	617.78	J/mol×K	750.08	Joback Method

dvisc	0.0196051	Pa×s	299.51	Joback Method
dvisc	0.0039450	Pa×s	347.22	Joback Method
dvisc	0.0011695	Pa×s	394.94	Joback Method
dvisc	0.0004506	Pa×s	442.65	Joback Method
dvisc	0.0002090	Pa×s	490.36	Joback Method
dvisc	0.0001111	Pa×s	538.08	Joback Method
dvisc	0.0000655	Pa×s	585.79	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1653378&Units=SI

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
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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