2-Methyldecan-2-ol

Inchi: InChI=1S/C11H24O/c1-4-5-6-7-8-9-10-11(2,3)12/h12H,4-10H2,1-3H3
InchiKey: WTXBAYPZJKPZHX-UHFFFAOYSA-N
Formula: C11H24O
SMILES: CCCCCCCCC(C)(C)O
Mol. weight [g/mol]: 172.31

Physical Properties

Property code	Value	Unit	Source
af	0.7479		Cheméo Relay (1.0)
gf	-92.24	kJ/mol	Joback Method
hf	-462.73	kJ/mol	Cheméo Relay (1.0)
hfus	20.92	kJ/mol	Joback Method
hvap	74.43	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
log10ws	-3.65		Cheméo Relay (1.0)
logp	3.508		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1230.70		NIST Webbook
rinpol	1230.70		NIST Webbook
tb	492.55	K	Cheméo Relay (1.0)
tc	666.18	K	Cheméo Relay (1.0)
tf	279.92	K	Cheméo Relay (1.0)
vc	0.663	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.60	J/mol×K	540.03	Joback Method
cpg	510.59	J/mol×K	705.71	Joback Method
cpg	498.91	J/mol×K	678.09	Joback Method
cpg	486.67	J/mol×K	650.48	Joback Method
cpg	473.84	J/mol×K	622.87	Joback Method
cpg	460.40	J/mol×K	595.26	Joback Method

cpg	446.33	J/mol×K	567.64	Joback Method
dvisc	0.0007039	Pa×s	408.50	Joback Method
dvisc	0.0000980	Pa×s	540.03	Joback Method
dvisc	0.0001684	Pa×s	496.19	Joback Method
dvisc	0.0003212	Pa×s	452.34	Joback Method
dvisc	0.0328701	Pa×s	276.97	Joback Method
dvisc	0.0018627	Pa×s	364.66	Joback Method
dvisc	0.0064311	Pa×s	320.81	Joback Method

Sources

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=C3396029&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

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume