OCTANE, 4,5-DIETHYL-

Other names: 4,5-diethyl-octane
Inchi: InChI=1S/C12H26/c1-5-9-11(7-3)12(8-4)10-6-2/h11-12H,5-10H2,1-4H3
InchiKey: XRVCHXCONYJHLU-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCCC(CC)C(CC)CCC
Mol. weight [g/mol]: 170.34

Physical Properties

Property code	Value	Unit	Source
af	0.4743		Cheméo Relay (1.0)
gf	45.28	kJ/mol	Joback Method
hf	-271.63	kJ/mol	Cheméo Relay (1.0)
hfus	19.79	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Cheméo Relay (1.0)
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-5.97		Cheméo Relay (1.0)
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1083.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1092.00		NIST Webbook
tb	466.00 ± 5.00	K	NIST Webbook
tc	633.58	K	Cheméo Relay (1.0)
tf	203.00 ± 3.00	K	NIST Webbook
vc	0.647	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.97	J/mol×K	473.08	Joback Method

cpg	502.54	J/mol×K	640.63	Joback Method
cpg	488.21	J/mol×K	612.70	Joback Method
cpg	473.26	J/mol×K	584.78	Joback Method
cpg	457.68	J/mol×K	556.85	Joback Method
cpg	441.45	J/mol×K	528.93	Joback Method
cpg	424.55	J/mol×K	501.00	Joback Method
dvisc	0.0007305	Pa×s	334.04	Joback Method
dvisc	0.0001925	Pa×s	473.08	Joback Method
dvisc	0.0002726	Pa×s	426.73	Joback Method
dvisc	0.0004202	Pa×s	380.39	Joback Method
dvisc	0.0185767	Pa×s	195.00	Joback Method
dvisc	0.0015175	Pa×s	287.69	Joback Method
dvisc	0.0041744	Pa×s	241.35	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=C1636415&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume