

3,6-diethyl-octane

Inchi:	InChI=1S/C12H26/c1-5-11(6-2)9-10-12(7-3)8-4/h11-12H,5-10H2,1-4H3
InchiKey:	UTCTYSTYZOAAOS-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCC(CC)CCC(CC)CC
Mol. weight [g/mol]:	170.33

Physical Properties

Property code	Value	Unit	Source
gf	45.28	kJ/mol	Joback Method
hf	-301.57	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	41.53	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1124.60		NIST Webbook
rinpol	1124.60		NIST Webbook
rinpol	1123.10		NIST Webbook
rinpol	1123.90		NIST Webbook
tb	473.08	K	Joback Method
tc	640.63	K	Joback Method
tf	195.00	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.97	J/molxK	473.08	Joback Method
cpg	424.55	J/molxK	501.00	Joback Method
cpg	441.45	J/molxK	528.93	Joback Method
cpg	457.68	J/molxK	556.85	Joback Method
cpg	473.26	J/molxK	584.78	Joback Method
cpg	488.21	J/molxK	612.70	Joback Method

cpg	502.54	J/mol×K	640.63	Joback Method
dvisc	0.0185767	Paxs	195.00	Joback Method
dvisc	0.0041744	Paxs	241.35	Joback Method
dvisc	0.0015175	Paxs	287.69	Joback Method
dvisc	0.0007305	Paxs	334.04	Joback Method
dvisc	0.0004202	Paxs	380.39	Joback Method
dvisc	0.0002726	Paxs	426.73	Joback Method
dvisc	0.0001925	Paxs	473.08	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R173203&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvap:	Enthalpy of vaporization at standard conditions
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

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