

Octane, 3-ethyl-2,7-dimethyl-

Other names:	3-Ethyl-2,7-dimethyl octane
Inchi:	InChI=1S/C12H26/c1-6-12(11(4)5)9-7-8-10(2)3/h10-12H,6-9H2,1-5H3
InchiKey:	XEMFRSYZKNPRTA-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCC(CCCC(C)C)C(C)C
Mol. weight [g/mol]:	170.33
CAS:	62183-55-5

Physical Properties

Property code	Value	Unit	Source
gf	42.84	kJ/mol	Joback Method
hf	-306.85	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	41.14	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.495		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	1180.00		NIST Webbook
tb	472.64	K	Joback Method
tc	643.64	K	Joback Method
tf	180.00	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.03	J/molxK	472.64	Joback Method
cpg	425.05	J/molxK	501.14	Joback Method
cpg	442.35	J/molxK	529.64	Joback Method
cpg	458.95	J/molxK	558.14	Joback Method
cpg	474.87	J/molxK	586.64	Joback Method
cpg	490.12	J/molxK	615.14	Joback Method
cpg	504.72	J/molxK	643.64	Joback Method

dvisc	0.0383167	Paxs	180.00	Joback Method
dvisc	0.0060831	Paxs	228.77	Joback Method
dvisc	0.0018440	Paxs	277.55	Joback Method
dvisc	0.0007987	Paxs	326.32	Joback Method
dvisc	0.0004300	Paxs	375.09	Joback Method
dvisc	0.0002670	Paxs	423.87	Joback Method
dvisc	0.0001829	Paxs	472.64	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=C62183555&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
mvol:	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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