

Octane, 3,7-dimethyl-1-(2,5-xylyl)-

Other names:	1,4-Dimethyl-2-(3,7-dimethyloctyl)benzene
Inchi:	InChI=1S/C18H30/c1-14(2)7-6-8-15(3)10-12-18-13-16(4)9-11-17(18)5/h9,11,13-15H,6-8,
InchiKey:	GDGPOTBJJLOPRZ-UHFFFAOYSA-N
Formula:	C18H30
SMILES:	<chem>Cc1ccc(C)c(CCC(C)CCCC(C)C)c1</chem>
Mol. weight [g/mol]:	246.43
CAS:	19550-60-8

Physical Properties

Property code	Value	Unit	Source
gf	188.95	kJ/mol	Joback Method
hf	-211.82	kJ/mol	Joback Method
hfus	28.59	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.698		Crippen Method
mcvol	240.720	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
tb	647.00	K	Joback Method
tc	840.66	K	Joback Method
tf	314.08	K	Joback Method
vc	0.923	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.92	J/molxK	647.00	Joback Method
cpg	745.49	J/molxK	808.39	Joback Method
cpg	729.30	J/molxK	776.11	Joback Method
cpg	712.19	J/molxK	743.83	Joback Method
cpg	694.11	J/molxK	711.55	Joback Method
cpg	675.03	J/molxK	679.28	Joback Method
cpg	760.78	J/molxK	840.66	Joback Method
dvisc	0.0001040	Paxs	647.00	Joback Method

dvisc	0.0001392	Paxs	591.51	Joback Method
dvisc	0.0001979	Paxs	536.03	Joback Method
dvisc	0.0003053	Paxs	480.54	Joback Method
dvisc	0.0005273	Paxs	425.05	Joback Method
dvisc	0.0010733	Paxs	369.57	Joback Method
dvisc	0.0028079	Paxs	314.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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