

Benzene, 1,3,5-trimethyl-2-octadecyl-

Other names:	1-(2,4,6-Trimethylphenyl)octadecane 1,3,5-Trimethyl-2-n-octadecylbenzene 2,4,6-Trimethyl-n-octadecylbenzene
Inchi:	InChI=1S/C27H48/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-27-25(3)22-24(2)
InchiKey:	SDJSEINVDXJJCL-UHFFFAOYSA-N
Formula:	C27H48
SMILES:	CCCCCCCCCCCCCCCCCc1c(C)cc(C)cc1C
Mol. weight [g/mol]:	372.67
CAS:	55282-67-2

Physical Properties

Property code	Value	Unit	Source
gf	259.98	kJ/mol	Joback Method
hf	-398.49	kJ/mol	Joback Method
hfus	58.56	kJ/mol	Joback Method
hvap	79.96	kJ/mol	Joback Method
log10ws	-10.40		Crippen Method
logp	9.416		Crippen Method
mcvol	367.530	ml/mol	McGowan Method
pc	805.25	kPa	Joback Method
tb	858.78	K	Joback Method
tc	1052.64	K	Joback Method
tf	327.55 ± 0.50	K	NIST Webbook
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1197.26	J/mol×K	858.78	Joback Method
cpg	1219.21	J/mol×K	891.09	Joback Method
cpg	1239.96	J/mol×K	923.40	Joback Method
cpg	1259.55	J/mol×K	955.71	Joback Method
cpg	1278.05	J/mol×K	988.02	Joback Method
cpg	1295.50	J/mol×K	1020.33	Joback Method

cpg	1311.95	J/mol×K	1052.64	Joback Method
dvisc	0.0006551	Pa×s	458.03	Joback Method
dvisc	0.0003066	Pa×s	524.82	Joback Method
dvisc	0.0001703	Pa×s	591.61	Joback Method
dvisc	0.0001066	Pa×s	658.40	Joback Method
dvisc	0.0000728	Pa×s	725.20	Joback Method
dvisc	0.0000529	Pa×s	791.99	Joback Method
dvisc	0.0000405	Pa×s	858.78	Joback Method

Sources

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=C55282672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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