

Benzene, 2-(1-decylundecyl)-1,4-dimethyl-

Other names:	11-(2,5-Dimethylphenyl)heneicosane 11-(2,5-Xylyl)heneicosane Heneicosane, 11-(2,5-dimethylphenyl)-
Inchi:	InChI=1S/C29H52/c1-5-7-9-11-13-15-17-19-21-28(29-25-26(3)23-24-27(29)4)22-20-18-1
InchiKey:	XDZKZNNMWLIULQ-UHFFFAOYSA-N
Formula:	C29H52
SMILES:	CCCCCCCCCCC(CCCCCCCCCC)c1cc(C)ccc1C
Mol. weight [g/mol]:	400.72
CAS:	55373-91-6

Physical Properties

Property code	Value	Unit	Source
gf	284.01	kJ/mol	Joback Method
hf	-433.58	kJ/mol	Joback Method
hfus	60.61	kJ/mol	Joback Method
hvap	83.36	kJ/mol	Joback Method
log10ws	-11.14		Crippen Method
logp	10.449		Crippen Method
mcvol	395.710	ml/mol	McGowan Method
pc	733.23	kPa	Joback Method
tb	899.12	K	Joback Method
tc	1100.78	K	Joback Method
tf	453.05	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.61	J/molxK	899.12	Joback Method
cpg	1349.50	J/molxK	932.73	Joback Method
cpg	1371.07	J/molxK	966.34	Joback Method
cpg	1391.37	J/molxK	999.95	Joback Method
cpg	1410.48	J/molxK	1033.56	Joback Method
cpg	1428.47	J/molxK	1067.17	Joback Method

cpg	1445.41	J/mol×K	1100.78	Joback Method
dvisc	0.0007419	Paxs	453.05	Joback Method
dvisc	0.0002908	Paxs	527.39	Joback Method
dvisc	0.0001437	Paxs	601.74	Joback Method
dvisc	0.0000829	Paxs	676.08	Joback Method
dvisc	0.0000533	Paxs	750.43	Joback Method
dvisc	0.0000372	Paxs	824.77	Joback Method
dvisc	0.0000275	Paxs	899.12	Joback Method
hvapt	100.80	kJ/mol	503.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55373916&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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