Benzene, (3-octylundecyl)-

Other names:	Heptadecane, 9-phenethyl-
	9-(2-Phenylethyl)heptadecane
	9-(2'-Phenylethyl)heptadecane
	3-Octyl-1-phenylundecane
Inchi:	InChI=1S/C25H44/c1-3-5-7-9-11-14-18-24(19-15-12-10-8-6-4-2)22-23-25-20-16-13-17-21
InchiKey:	YFDREPVYVBGJDD-UHFFFAOYSA-N
Formula:	C25H44
SMILES:	CCCCCCCCC(CCCCCCCC)CCc1ccccc1
Mol. weight [g/mol]:	344.62
CAS:	5637-96-7

Physical Properties

Property code	Value	Unit	Source
gf	269.59	kJ/mol	Joback Method
hf	-328.08	kJ/mol	Joback Method
hfus	51.02	kJ/mol	Joback Method
hvap	73.13	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	8.737		Crippen Method
mcvol	339.350	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
tb	797.64	K	Joback Method
tc	984.29	K	Joback Method
tf	246.45 ± 0.50	K	NIST Webbook
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.77	J/mol×K	797.64	Joback Method
cpg	1091.37	J/mol×K	828.75	Joback Method
cpg	1111.81	J/mol×K	859.86	Joback Method
cpg	1131.16	J/mol×K	890.96	Joback Method
cpg	1149.47	J/mol×K	922.07	Joback Method

cpg	1166.78	J/mol×K	953.18	Joback Method
cpg	1183.17	J/mol×K	984.29	Joback Method
dvisc	0.0006485	Pa×s	452.05	Joback Method
dvisc	0.0019334	Pa×s	382.93	Joback Method
dvisc	0.0002906	Pa×s	521.17	Joback Method
dvisc	0.0001572	Pa×s	590.28	Joback Method
dvisc	0.0000967	Pa×s	659.40	Joback Method
dvisc	0.0000652	Pa×s	728.52	Joback Method
dvisc	0.0000471	Pa×s	797.64	Joback Method
hvapt	89.40	kJ/mol	494.50	NIST Webbook
hvapt	88.30	kJ/mol	480.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5637967&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume