Tridecane, 2,2,4,10,12,12-hexamethyl-7-(3,5,5-trimethylhexyl)

Other names: 2,2,4,10,12,12-Hexamethyl-7-(3,5,5-trimethylhexyl)tridecane
Inchi: InChI=1S/C28H58/c1-22(19-26(4,5)6)13-16-25(17-14-23(2)20-27(7,8)9)18-15-24(3)21-28
InchiKey: VJDJSJSGMRWTIK-UHFFFAOYSA-N
Formula: C28H58
SMILES: CC(CCC(CCC(C)CC(C)(C)C)CCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 394.76
CAS: 3035-75-4

Physical Properties

Property code	Value	Unit	Source
gf	183.64	kJ/mol	Joback Method
hf	-668.62	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	10.160		Crippen Method
mcvol	405.380	ml/mol	McGowan Method
pc	686.37	kPa	Joback Method
tb	828.59	K	Joback Method
tc	1018.55	K	Joback Method
tf	352.58	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.27	J/mol×K	986.89	Joback Method
cpg	1481.73	J/mol×K	1018.55	Joback Method
cpg	1349.63	J/mol×K	828.59	Joback Method
cpg	1374.54	J/mol×K	860.25	Joback Method
cpg	1398.15	J/mol×K	891.91	Joback Method
cpg	1420.58	J/mol×K	923.57	Joback Method
cpg	1441.92	J/mol×K	955.23	Joback Method
dvisc	0.0000116	Pa×s	828.59	Joback Method

dvisc	0.0000189	Pa×s	749.25	Joback Method
dvisc	0.0058590	Pa×s	352.58	Joback Method
dvisc	0.0008009	Pa×s	431.91	Joback Method
dvisc	0.0002030	Pa×s	511.25	Joback Method
dvisc	0.0000744	Pa×s	590.59	Joback Method
dvisc	0.0000346	Pa×s	669.92	Joback Method
hvapt	84.90	kJ/mol	460.00	NIST Webbook
hvapt	98.50	kJ/mol	350.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66252e+01
Coeff. B	-6.64497e+03
Coeff. C	-1.37070e+02
Temperature range (K), min.	543.80
Temperature range (K), max.	724.41

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3035754&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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