6-Tridecene, 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)-6-tridecene
Inchi: InChI=1S/C28H56/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: NWNPVUYOZGIYLE-UHFFFAOYSA-N
Formula: C28H56
SMILES: CC(CC=C(CCC(C)CC(C)(C)C)CCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 392.74
CAS: 55255-73-7

Physical Properties

Property code	Value	Unit	Source
gf	257.75	kJ/mol	Joback Method
hf	-555.91	kJ/mol	Joback Method
hfus	34.36	kJ/mol	Joback Method
hvap	72.91	kJ/mol	Joback Method
log10ws	-9.95		Crippen Method
logp	10.080		Crippen Method
mcvol	401.080	ml/mol	McGowan Method
pc	704.33	kPa	Joback Method
tb	833.07	K	Joback Method
tc	1025.75	K	Joback Method
tf	348.54	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1323.91	J/mol×K	833.07	Joback Method
cpg	1348.35	J/mol×K	865.18	Joback Method
cpg	1371.58	J/mol×K	897.30	Joback Method
cpg	1393.71	J/mol×K	929.41	Joback Method
cpg	1414.85	J/mol×K	961.52	Joback Method
cpg	1435.12	J/mol×K	993.64	Joback Method
cpg	1454.63	J/mol×K	1025.75	Joback Method
hvapt	83.80	kJ/mol	457.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43155e+01
Coeff. B	-6.67194e+03
Coeff. C	-1.25050e+01
Temperature range (K), min.	488.13
Temperature range (K), max.	753.50

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55255737&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

Legend

cpg:	Ideal gas heat capacity
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