

Pyrene, 1-decylohexadecahydro-

Other names:	3-n-Decyl-(hexadecahydropyrene) 3-n-Decylperhydropyrene
Inchi:	InChI=1S/C26H46/c1-2-3-4-5-6-7-8-9-11-20-14-15-23-17-16-21-12-10-13-22-18-19-24(2
InchiKey:	DEVZYFUPAIBVPP-UHFFFAOYSA-N
Formula:	C26H46
SMILES:	CCCCCCCCCCC1CCC2CCC3CCCC4CCC1C2C34
Mol. weight [g/mol]:	358.64
CAS:	55191-41-8

Physical Properties

Property code	Value	Unit	Source
gf	339.51	kJ/mol	Joback Method
hf	-374.43	kJ/mol	Joback Method
hfus	50.45	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	8.396		Crippen Method
mvol	333.760	ml/mol	McGowan Method
pc	980.85	kPa	Joback Method
tb	824.31	K	Joback Method
tc	1028.20	K	Joback Method
tf	427.74	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1185.96	J/molxK	824.31	Joback Method
cpg	1212.22	J/molxK	858.29	Joback Method
cpg	1236.97	J/molxK	892.27	Joback Method
cpg	1260.32	J/molxK	926.26	Joback Method
cpg	1282.39	J/molxK	960.24	Joback Method
cpg	1303.29	J/molxK	994.22	Joback Method
cpg	1323.14	J/molxK	1028.20	Joback Method

dvisc	0.0046488	Paxs	427.74	Joback Method
dvisc	0.0036130	Paxs	493.83	Joback Method
dvisc	0.0029801	Paxs	559.93	Joback Method
dvisc	0.0025601	Paxs	626.02	Joback Method
dvisc	0.0022640	Paxs	692.12	Joback Method
dvisc	0.0020456	Paxs	758.21	Joback Method
dvisc	0.0018785	Paxs	824.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55191418&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
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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