

12-Propyltricosane

Inchi:	InChI=1S/C26H54/c1-4-7-9-11-13-15-17-19-21-24-26(23-6-3)25-22-20-18-16-14-12-10-8
InchiKey:	IGKRUVDUCXLMHO-UHFFFAOYSA-N
Formula:	C26H54
SMILES:	CCCCCCCCCCCC(CCC)CCCCCCCCCCCC
Mol. weight [g/mol]:	366.71
CAS:	79370-84-6

Physical Properties

Property code	Value	Unit	Source
af	1.0150		Cheméo Relay (1.0)
gf	165.60	kJ/mol	Joback Method
hf	-578.01	kJ/mol	Cheméo Relay (1.0)
hfus	59.57	kJ/mol	Joback Method
hvap	121.12	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
log10ws	-10.18		Cheméo Relay (1.0)
logp	10.244		Crippen Method
mcvol	377.200	ml/mol	McGowan Method
pc	728.10	kPa	Joback Method
tb	616.22	K	Cheméo Relay (1.0)
tc	785.41	K	Cheméo Relay (1.0)
tf	276.71	K	Cheméo Relay (1.0)
vc	1.467	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1216.69	J/mol×K	793.84	Joback Method
cpg	1240.72	J/mol×K	823.53	Joback Method
cpg	1263.59	J/mol×K	853.21	Joback Method
cpg	1285.35	J/mol×K	882.90	Joback Method
cpg	1306.05	J/mol×K	912.59	Joback Method
cpg	1325.72	J/mol×K	942.27	Joback Method
cpg	1344.42	J/mol×K	971.96	Joback Method

dvisc	0.0023771	Pa×s	367.78	Joback Method
dvisc	0.0006945	Pa×s	438.79	Joback Method
dvisc	0.0002858	Pa×s	509.80	Joback Method
dvisc	0.0001462	Pa×s	580.81	Joback Method
dvisc	0.0000865	Pa×s	651.82	Joback Method
dvisc	0.0000568	Pa×s	722.83	Joback Method
dvisc	0.0000402	Pa×s	793.84	Joback Method
hvapt	91.00	kJ/mol	444.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56158e+01
Coeff. B	-5.95640e+03
Coeff. C	-1.27410e+02
Temperature range (K), min.	516.00
Temperature range (K), max.	705.46

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79370846&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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