1-PENTACOSANOL

Other names: pentacosyl alcohol
Inchi: InChI=1S/C25H52O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-
InchiKey: IACKKVBKKNJZGN-UHFFFAOYSA-N
Formula: C25H52O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]: 368.69
CAS: 26040-98-2

Physical Properties

Property code	Value	Unit	Source
af	1.3079		Cheméo Relay (1.0)
gf	22.80	kJ/mol	Joback Method
hf	-724.93	kJ/mol	Cheméo Relay (1.0)
hfus	64.59	kJ/mol	Joback Method
hvap	156.07	kJ/mol	Cheméo Relay (1.0)
ie	10.31	eV	Cheméo Relay (1.0)
log10ws	-8.93		Cheméo Relay (1.0)
logp	8.971		Crippen Method
mcvol	368.980	ml/mol	McGowan Method
pc	804.33	kPa	Joback Method
tb	643.51	K	Cheméo Relay (1.0)
tc	826.14	K	Cheméo Relay (1.0)
tf	351.15	K	Cheméo Relay (1.0)
vc	1.466	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1240.65	J/mol×K	863.58	Joback Method
cpg	1361.13	J/mol×K	1061.84	Joback Method
cpg	1343.74	J/mol×K	1028.79	Joback Method
cpg	1325.35	J/mol×K	995.75	Joback Method
cpg	1305.91	J/mol×K	962.71	Joback Method
cpg	1285.36	J/mol×K	929.67	Joback Method

cpg	1263.63	J/mol×K	896.62	Joback Method
dvisc	0.0000420	Pa×s	647.96	Joback Method
dvisc	0.0000078	Pa×s	863.58	Joback Method
dvisc	0.0000123	Pa×s	791.71	Joback Method
dvisc	0.0000214	Pa×s	719.83	Joback Method
dvisc	0.0012265	Pa×s	432.33	Joback Method
dvisc	0.0000977	Pa×s	576.08	Joback Method
dvisc	0.0002890	Pa×s	504.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46157e+01
Coeff. B	-5.72452e+03
Coeff. C	-1.29509e+02
Temperature range (K), min.	529.04
Temperature range (K), max.	744.77

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26040982&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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