14-Heptacosanone

Other names: Ditridecyl ketone
heptacosan-14-one
Inchi: InChI=1S/C27H54O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27(28)26-24-22-20-18-16-14-1
InchiKey: VCZMOZVQLARCOE-UHFFFAOYSA-N
Formula: C27H54O
SMILES: CCCCCCCCCCCCCC(=O)CCCCCCCCCCCCC
Mol. weight [g/mol]: 394.72
CAS: 542-50-7

Physical Properties

Property code	Value	Unit	Source
gf	47.54	kJ/mol	Joback Method
hf	-713.19	kJ/mol	Joback Method
hfus	67.28	kJ/mol	Joback Method
hvap	82.44	kJ/mol	Joback Method
log10ws	-10.40		Crippen Method
logp	9.958		Crippen Method
mcvol	392.860	ml/mol	McGowan Method
pc	712.25	kPa	Joback Method
tb	871.03	K	Joback Method
tc	1068.20	K	Joback Method
tf	443.98	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.68	J/mol×K	871.03	Joback Method
cpg	1339.36	J/mol×K	903.89	Joback Method
cpg	1361.73	J/mol×K	936.75	Joback Method
cpg	1382.84	J/mol×K	969.62	Joback Method
cpg	1402.77	J/mol×K	1002.48	Joback Method
cpg	1421.57	J/mol×K	1035.34	Joback Method
cpg	1439.30	J/mol×K	1068.20	Joback Method

dvisc	0.0011050	Pa×s	443.98	Joback Method
dvisc	0.0004213	Pa×s	515.15	Joback Method
dvisc	0.0002030	Pa×s	586.33	Joback Method
dvisc	0.0001145	Pa×s	657.50	Joback Method
dvisc	0.0000723	Pa×s	728.68	Joback Method
dvisc	0.0000495	Pa×s	799.86	Joback Method
dvisc	0.0000361	Pa×s	871.03	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65724e+01
Coeff. B	-6.83660e+03
Coeff. C	-1.45105e+02
Temperature range (K), min.	564.92
Temperature range (K), max.	752.21

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=C542507&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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume