Octacosanal

Inchi: InChI=1S/C28H56O/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: LVXORIXZNUNHGQ-UHFFFAOYSA-N
Formula: C28H56O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]: 408.75

Physical Properties

Property code	Value	Unit	Source
af	1.2164		Cheméo Relay (1.0)
gf	85.36	kJ/mol	Joback Method
hf	-726.50	kJ/mol	Cheméo Relay (1.0)
hfus	70.57	kJ/mol	Joback Method
hvap	147.50	kJ/mol	Cheméo Relay (1.0)
ie	10.13	eV	Cheméo Relay (1.0)
log10ws	-9.73		Cheméo Relay (1.0)
logp	10.348		Crippen Method
mcvol	406.950	ml/mol	McGowan Method
pc	681.00	kPa	Joback Method
rinpol	3014.00		NIST Webbook
rinpol	3032.00		NIST Webbook
rinpol	3039.70		NIST Webbook
rinpol	3039.70		NIST Webbook
rinpol	3014.00		NIST Webbook
tb	649.30	K	Cheméo Relay (1.0)
tc	840.33	K	Cheméo Relay (1.0)
tf	349.67	K	Cheméo Relay (1.0)
vc	1.611	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.36	J/mol×K	888.70	Joback Method
cpg	1403.96	J/mol×K	922.75	Joback Method
cpg	1427.14	J/mol×K	956.79	Joback Method

cpg	1448.99	J/mol×K	990.84	Joback Method
cpg	1469.59	J/mol×K	1024.89	Joback Method
cpg	1489.01	J/mol×K	1058.93	Joback Method
cpg	1507.33	J/mol×K	1092.98	Joback Method
dvisc	0.0011405	Pa×s	447.32	Joback Method
dvisc	0.0004233	Pa×s	520.88	Joback Method
dvisc	0.0002008	Pa×s	594.45	Joback Method
dvisc	0.0001122	Pa×s	668.01	Joback Method
dvisc	0.0000704	Pa×s	741.57	Joback Method
dvisc	0.0000480	Pa×s	815.14	Joback Method
dvisc	0.0000349	Pa×s	888.70	Joback Method

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22725640&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume