Hexacosanal

Inchi: InChI=1S/C26H52O/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: QAXXQMIHMLTJQI-UHFFFAOYSA-N
Formula: C26H52O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]: 380.70

Physical Properties

Property code	Value	Unit	Source
af	1.1463		Cheméo Relay (1.0)
gf	68.52	kJ/mol	Joback Method
hf	-685.20	kJ/mol	Cheméo Relay (1.0)
hfus	65.39	kJ/mol	Joback Method
hvap	137.82	kJ/mol	Cheméo Relay (1.0)
ie	10.06	eV	Cheméo Relay (1.0)
log10ws	-9.18		Cheméo Relay (1.0)
logp	9.568		Crippen Method
mcvol	378.770	ml/mol	McGowan Method
pc	754.74	kPa	Joback Method
rinpol	2830.00		NIST Webbook
rinpol	2815.00		NIST Webbook
rinpol	2833.50		NIST Webbook
tb	636.87	K	Cheméo Relay (1.0)
tc	828.01	K	Cheméo Relay (1.0)
tf	345.89	K	Cheméo Relay (1.0)
vc	1.501	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.68	J/mol×K	842.94	Joback Method
cpg	1369.56	J/mol×K	1032.67	Joback Method
cpg	1352.07	J/mol×K	1001.05	Joback Method
cpg	1333.59	J/mol×K	969.43	Joback Method
cpg	1314.07	J/mol×K	937.80	Joback Method

cpg	1293.45	J/mol×K	906.18	Joback Method
cpg	1271.67	J/mol×K	874.56	Joback Method
dvisc	0.0001489	Pa×s	633.86	Joback Method
dvisc	0.0000469	Pa×s	842.94	Joback Method
dvisc	0.0000643	Pa×s	773.25	Joback Method
dvisc	0.0000939	Pa×s	703.55	Joback Method
dvisc	0.0014732	Pa×s	424.78	Joback Method
dvisc	0.0002647	Pa×s	564.17	Joback Method
dvisc	0.0005533	Pa×s	494.47	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26627850&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):

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