11,16-didecylhexacosane

Other names: 11,16-didecylhexacosane
Inchi: InChI=1S/C46H94/c1-5-9-13-17-21-25-29-33-39-45(40-34-30-26-22-18-14-10-6-2)43-37-
InchiKey: DJOOEZMZUMXNFD-UHFFFAOYSA-N
Formula: C46H94
SMILES: CCCCCCCCCCC(CCCCCCCCCC)CCCCC(CCCCCCCCCC)CCCCCCCCCC
Mol. weight [g/mol]: 647.24
CAS: 500016-84-2

Physical Properties

Property code	Value	Unit	Source
af	1.6523		Cheméo Relay (1.0)
gf	331.56	kJ/mol	Joback Method
hf	-1016.39	kJ/mol	Cheméo Relay (1.0)
hfus	107.85	kJ/mol	Joback Method
hvap	207.20	kJ/mol	Cheméo Relay (1.0)
ie	10.39	eV	Cheméo Relay (1.0)
log10ws	-15.47		Cheméo Relay (1.0)
logp	17.902		Crippen Method
mcvol	659.000	ml/mol	McGowan Method
pc	316.84	kPa	Joback Method
tb	746.44	K	Cheméo Relay (1.0)
tc	898.63	K	Cheméo Relay (1.0)
tf	319.40 ± 0.80	K	NIST Webbook
tf	321.20 ± 0.50	K	NIST Webbook
vc	2.536	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2602.99	J/mol×K	1251.00	Joback Method
cpg	2938.52	J/mol×K	1825.60	Joback Method
cpg	2878.59	J/mol×K	1729.83	Joback Method
cpg	2824.03	J/mol×K	1634.07	Joback Method
cpg	2772.00	J/mol×K	1538.30	Joback Method

cpg	2719.70	J/mol×K	1442.53	Joback Method
cpg	2664.31	J/mol×K	1346.77	Joback Method
dvisc	0.0000059	Pa×s	914.59	Joback Method
dvisc	0.0000015	Pa×s	1251.00	Joback Method
dvisc	0.0000022	Pa×s	1138.86	Joback Method
dvisc	0.0000034	Pa×s	1026.73	Joback Method
dvisc	0.0001195	Pa×s	578.18	Joback Method
dvisc	0.0000122	Pa×s	802.45	Joback Method
dvisc	0.0000318	Pa×s	690.32	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C500016842&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

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