3,4-Diethyl-3,4-dimethoxyhexane

Inchi: InChI=1S/C12H26O2/c1-7-11(8-2,13-5)12(9-3,10-4)14-6/h7-10H2,1-6H3
InchiKey: KGFJBMIBGUJGSB-UHFFFAOYSA-N
Formula: C12H26O2
SMILES: CCC(CC)(OC)C(CC)(CC)OC
Mol. weight [g/mol]: 202.33
CAS: 125379-19-3

Physical Properties

Property code	Value	Unit	Source
chl	-7866.00 ± 3.00	kJ/mol	NIST Webbook
gf	-154.16	kJ/mol	Joback Method
hf	-512.00 ± 3.00	kJ/mol	NIST Webbook
hfus	14.38	kJ/mol	Joback Method
hvap	44.53	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.397		Crippen Method
mcvol	191.680	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
tb	512.34	K	Joback Method
tc	691.40	K	Joback Method
tf	274.30	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.49	J/mol×K	691.40	Joback Method
cpg	553.13	J/mol×K	661.56	Joback Method
cpg	538.02	J/mol×K	631.71	Joback Method
cpg	522.13	J/mol×K	601.87	Joback Method
cpg	505.43	J/mol×K	572.03	Joback Method
cpg	487.91	J/mol×K	542.18	Joback Method
cpg	469.53	J/mol×K	512.34	Joback Method
dvisc	0.0051695	Pa×s	274.30	Joback Method

dvisc	0.0001319	Pa×s	512.34	Joback Method
dvisc	0.0001881	Pa×s	472.67	Joback Method
dvisc	0.0002863	Pa×s	432.99	Joback Method
dvisc	0.0004741	Pa×s	393.32	Joback Method
dvisc	0.0008793	Pa×s	353.65	Joback Method
dvisc	0.0019063	Pa×s	313.97	Joback Method
hvapt	60.00 ± 1.00	kJ/mol	302.20	NIST Webbook

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=C125379193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
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

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