dodecyl octyl ether

Inchi: InChI=1S/C20H42O/c1-3-5-7-9-11-12-13-14-16-18-20-21-19-17-15-10-8-6-4-2/h3-20H2,1
InchiKey: MMMPXNOKIZOWHM-UHFFFAOYSA-N
Formula: C20H42O
SMILES: CCCCCCCCCCCCOCCCCCCCC
Mol. weight [g/mol]: 298.55
CAS: 36339-51-2

Physical Properties

Property code	Value	Unit	Source
af	0.9209		Cheméo Relay (1.0)
gf	12.52	kJ/mol	Joback Method
hf	-586.81	kJ/mol	Cheméo Relay (1.0)
hfus	48.74	kJ/mol	Joback Method
hvap	98.79	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-7.50		Cheméo Relay (1.0)
logp	7.284		Crippen Method
mcvol	298.530	ml/mol	McGowan Method
pc	1004.62	kPa	Joback Method
tb	628.20 ± 2.00	K	NIST Webbook
tc	761.50	K	Cheméo Relay (1.0)
tf	279.00 ± 1.50	K	NIST Webbook
vc	1.189	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.71	J/mol×K	679.42	Joback Method
cpg	895.45	J/mol×K	706.44	Joback Method
cpg	915.33	J/mol×K	733.46	Joback Method
cpg	934.37	J/mol×K	760.49	Joback Method
cpg	952.59	J/mol×K	787.51	Joback Method
cpg	970.01	J/mol×K	814.53	Joback Method
cpg	986.65	J/mol×K	841.55	Joback Method

dvisc	0.0023688	Pa×s	337.39	Joback Method
dvisc	0.0008784	Pa×s	394.39	Joback Method
dvisc	0.0004185	Pa×s	451.40	Joback Method
dvisc	0.0002354	Pa×s	508.40	Joback Method
dvisc	0.0001487	Pa×s	565.41	Joback Method
dvisc	0.0001022	Pa×s	622.41	Joback Method
dvisc	0.0000748	Pa×s	679.42	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36339512&Units=SI

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

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