

Eicosyl octyl ether

Inchi:	InChI=1S/C28H58O/c1-3-5-7-9-11-12-13-14-15-16-17-18-19-20-21-22-24-26-28-29-27-2
InchiKey:	JRWROQIFZUYCIY-UHFFFAOYSA-N
Formula:	C28H58O
SMILES:	CCCCCCCCCCCCCCCCCCCCOCCCCCCCC
Mol. weight [g/mol]:	410.76

Physical Properties

Property code	Value	Unit	Source
gf	79.88	kJ/mol	Joback Method
hf	-753.47	kJ/mol	Joback Method
hfus	69.46	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-10.63		Crippen Method
logp	10.405		Crippen Method
mcvol	411.250	ml/mol	McGowan Method
pc	649.78	kPa	Joback Method
rinpol	2860.00		NIST Webbook
rinpol	2860.00		NIST Webbook
tb	862.46	K	Joback Method
tc	1059.66	K	Joback Method
tf	427.55	K	Joback Method
vc	1.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.56	J/molxK	862.46	Joback Method
cpg	1410.17	J/molxK	895.33	Joback Method
cpg	1434.34	J/molxK	928.19	Joback Method
cpg	1457.12	J/molxK	961.06	Joback Method
cpg	1478.56	J/molxK	993.93	Joback Method
cpg	1498.72	J/molxK	1026.79	Joback Method
cpg	1517.66	J/molxK	1059.66	Joback Method
dvisc	0.0009084	Paxs	427.55	Joback Method

dvisc	0.0003209	Paxs	500.03	Joback Method
dvisc	0.0001475	Paxs	572.52	Joback Method
dvisc	0.0000808	Paxs	645.00	Joback Method
dvisc	0.0000499	Paxs	717.49	Joback Method
dvisc	0.0000337	Paxs	789.98	Joback Method
dvisc	0.0000243	Paxs	862.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U406388&Units=SI

Legend

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
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

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