

Eicosyl ethyl ether

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C22H46O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-4-2/h3-

PRGOMPHKWHPFFI-UHFFFAOYSA-N

C22H46O

CCCCCCCCCCCCCCCCCCCCOCC

326.60

Physical Properties

Property code	Value	Unit	Source
gf	29.36	kJ/mol	Joback Method
hf	-629.63	kJ/mol	Joback Method
hfus	53.92	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	8.065		Crippen Method
mcvol	326.710	ml/mol	McGowan Method
pc	892.67	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	725.18	K	Joback Method
tc	891.69	K	Joback Method
tf	359.93	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.15	J/mol×K	725.18	Joback Method
cpg	1018.84	J/mol×K	752.93	Joback Method
cpg	1039.58	J/mol×K	780.68	Joback Method
cpg	1059.40	J/mol×K	808.43	Joback Method
cpg	1078.30	J/mol×K	836.19	Joback Method
cpg	1096.33	J/mol×K	863.94	Joback Method
cpg	1113.50	J/mol×K	891.69	Joback Method
dvisc	0.0019109	Pa×s	359.93	Joback Method

dvisc	0.0006985	Pa×s	420.80	Joback Method
dvisc	0.0003293	Pa×s	481.68	Joback Method
dvisc	0.0001837	Pa×s	542.55	Joback Method
dvisc	0.0001153	Pa×s	603.43	Joback Method
dvisc	0.0000789	Pa×s	664.30	Joback Method
dvisc	0.0000575	Pa×s	725.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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