

Eicosyl isobutyl ether

Inchi:

InChI=1S/C24H50O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-23-24(2

InchiKey:

GOCHXPOMSUKLRG-UHFFFAOYSA-N

Formula:

C24H50O

SMILES:

CCCCCCCCCCCCCCCCCCCCOCC(C)C

Mol. weight [g/mol]:

354.65

Physical Properties

Property code	Value	Unit	Source
gf	43.76	kJ/mol	Joback Method
hf	-676.19	kJ/mol	Joback Method
hfus	55.58	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.701		Crippen Method
mcvol	354.890	ml/mol	McGowan Method
pc	802.06	kPa	Joback Method
rinpol	2426.00		NIST Webbook
tb	770.50	K	Joback Method
tc	944.28	K	Joback Method
tf	367.47	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.71	J/mol×K	770.50	Joback Method
cpg	1146.54	J/mol×K	799.46	Joback Method
cpg	1168.29	J/mol×K	828.43	Joback Method
cpg	1188.99	J/mol×K	857.39	Joback Method
cpg	1208.66	J/mol×K	886.35	Joback Method
cpg	1227.33	J/mol×K	915.32	Joback Method
cpg	1245.05	J/mol×K	944.28	Joback Method
dvisc	0.0019554	Pa×s	367.47	Joback Method
dvisc	0.0006203	Pa×s	434.64	Joback Method

dvisc	0.0002676	Pa×s	501.81	Joback Method
dvisc	0.0001408	Pa×s	568.98	Joback Method
dvisc	0.0000848	Pa×s	636.16	Joback Method
dvisc	0.0000563	Pa×s	703.33	Joback Method
dvisc	0.0000401	Pa×s	770.50	Joback Method

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=U406330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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