

Eicosyl isopropyl ether

Inchi:	InChI=1S/C23H48O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24-23(2)3
InchiKey:	UBZGFZFEZYNVAV-UHFFFAOYSA-N
Formula:	C23H48O
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(C)C
Mol. weight [g/mol]:	340.63

Physical Properties

Property code	Value	Unit	Source
gf	35.34	kJ/mol	Joback Method
hf	-655.55	kJ/mol	Joback Method
hfus	52.99	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	8.453		Crippen Method
mcvol	340.800	ml/mol	McGowan Method
pc	847.51	kPa	Joback Method
rinpol	2326.00		NIST Webbook
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tb	747.62	K	Joback Method
tc	917.87	K	Joback Method
tf	356.20	K	Joback Method
vc	1.335	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1060.19	J/molxK	747.62	Joback Method
cpg	1082.51	J/molxK	776.00	Joback Method
cpg	1103.80	J/molxK	804.37	Joback Method
cpg	1124.10	J/molxK	832.75	Joback Method
cpg	1143.42	J/molxK	861.12	Joback Method
cpg	1161.81	J/molxK	889.50	Joback Method
cpg	1179.28	J/molxK	917.87	Joback Method
dvisc	0.0022255	Paxs	356.20	Joback Method

dvisc	0.0007078	Paxs	421.44	Joback Method
dvisc	0.0003061	Paxs	486.67	Joback Method
dvisc	0.0001613	Paxs	551.91	Joback Method
dvisc	0.0000974	Paxs	617.15	Joback Method
dvisc	0.0000647	Paxs	682.38	Joback Method
dvisc	0.0000462	Paxs	747.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406343&Units=SI
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

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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