

Cyclohexanecarboxylic acid, 4-methoxy-, dodecyl ester

Inchi:	InChI=1S/C20H38O3/c1-3-4-5-6-7-8-9-10-11-12-17-23-20(21)18-13-15-19(22-2)16-14-18
InchiKey:	JNAHGXAZZOAPEA-UHFFFAOYSA-N
Formula:	C20H38O3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	326.51

Physical Properties

Property code	Value	Unit	Source
gf	-204.66	kJ/mol	Joback Method
hf	-799.17	kJ/mol	Joback Method
hfus	44.44	kJ/mol	Joback Method
hvap	71.80	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.656		Crippen Method
mvol	295.110	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
tb	770.59	K	Joback Method
tc	957.71	K	Joback Method
tf	412.69	K	Joback Method
vc	1.129	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.95	J/molxK	770.59	Joback Method
cpg	1035.20	J/molxK	926.52	Joback Method
cpg	1018.95	J/molxK	895.34	Joback Method
cpg	1001.52	J/molxK	864.15	Joback Method
cpg	982.88	J/molxK	832.96	Joback Method
cpg	963.03	J/molxK	801.78	Joback Method
cpg	1050.28	J/molxK	957.71	Joback Method
dvisc	0.0000727	Paxs	770.59	Joback Method

dvisc	0.0000960	Paxs	710.94	Joback Method
dvisc	0.0001336	Paxs	651.29	Joback Method
dvisc	0.0001985	Paxs	591.64	Joback Method
dvisc	0.0003225	Paxs	531.99	Joback Method
dvisc	0.0005923	Paxs	472.34	Joback Method
dvisc	0.0012968	Paxs	412.69	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=U406200&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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