1,2-Cyclohexanedicarboxylic acid, dodecyl 2-ethoxyethyl ester

Inchi: InChI=1S/C24H44O5/c1-3-5-6-7-8-9-10-11-12-15-18-28-23(25)21-16-13-14-17-22(21)24

InchiKey: YZCYCYWMGNQKQI-UHFFFAOYSA-N

Formula: C24H44O5

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC

Mol. weight [g/mol]: 412.60

Physical Properties

Property code	Value	Unit	Source
gf	-404.90	kJ/mol	Joback Method
hf	-1126.53	kJ/mol	Joback Method
hfus	57.58	kJ/mol	Joback Method
hvap	89.86	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.837		Crippen Method
mcvol	358.910	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	2795.00		NIST Webbook
rinpol	2795.00		NIST Webbook
tb	938.40	K	Joback Method
tc	1148.87	K	Joback Method
tf	529.93	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.49	J/mol×K	938.40	Joback Method
cpg	1269.55	J/mol×K	973.48	Joback Method
cpg	1286.84	J/mol×K	1008.56	Joback Method
cpg	1302.36	J/mol×K	1043.63	Joback Method
cpg	1316.14	J/mol×K	1078.71	Joback Method
cpg	1328.20	J/mol×K	1113.79	Joback Method
cpg	1338.56	J/mol×K	1148.87	Joback Method
dvisc	0.0004466	Pa×s	529.93	Joback Method

dvisc	0.0002195	Pa×s	598.01	Joback Method
dvisc	0.0001248	Pa×s	666.09	Joback Method
dvisc	0.0000788	Pa×s	734.16	Joback Method
dvisc	0.0000538	Pa×s	802.24	Joback Method
dvisc	0.0000389	Pa×s	870.32	Joback Method
dvisc	0.0000296	Pa×s	938.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339914&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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