1,2-Cyclohexanedicarboxylic acid, decyl 5-methoxy-3-methylpentyl ester

Inchi: InChI=1S/C25H46O5/c1-4-5-6-7-8-9-10-13-18-29-24(26)22-14-11-12-15-23(22)25(27)30
InchiKey: VSCUVLUORPXHOY-UHFFFAOYSA-N
Formula: C25H46O5
SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC(C)CCOC
Mol. weight [g/mol]: 426.63

Physical Properties

Property code	Value	Unit	Source
gf	-398.92	kJ/mol	Joback Method
hf	-1152.45	kJ/mol	Joback Method
hfus	56.65	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	6.083		Crippen Method
mcvol	373.000	ml/mol	McGowan Method
pc	884.19	kPa	Joback Method
rinpol	2861.00		NIST Webbook
rinpol	2861.00		NIST Webbook
tb	960.84	K	Joback Method
tc	1176.57	K	Joback Method
tf	526.20	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1314.20	J/mol×K	960.84	Joback Method
cpg	1333.30	J/mol×K	996.80	Joback Method
cpg	1350.49	J/mol×K	1032.75	Joback Method
cpg	1365.78	J/mol×K	1068.71	Joback Method
cpg	1379.20	J/mol×K	1104.66	Joback Method
cpg	1390.78	J/mol×K	1140.62	Joback Method
cpg	1400.53	J/mol×K	1176.57	Joback Method
dvisc	0.0004446	Pa×s	526.20	Joback Method

dvisc	0.0002017	Pa×s	598.64	Joback Method
dvisc	0.0001085	Pa×s	671.08	Joback Method
dvisc	0.0000659	Pa×s	743.52	Joback Method
dvisc	0.0000437	Pa×s	815.96	Joback Method
dvisc	0.0000310	Pa×s	888.40	Joback Method
dvisc	0.0000232	Pa×s	960.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339922&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

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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