1,2-Cyclohexanedicarboxylic acid, dodecyl 3-pentyl ester

Inchi: InChI=1S/C25H46O4/c1-4-7-8-9-10-11-12-13-14-17-20-28-24(26)22-18-15-16-19-23(22)25(27)29-21(5-2)6-3/h21-23H,4-20H2,1-3H3

InchiKey: SRBLDMUDXFCXIU-UHFFFAOYSA-N

Formula: C25H46O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)CC

Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-293.92	kJ/mol	Joback Method
hf	-1020.23	kJ/mol	Joback Method
hfus	55.46	kJ/mol	Joback Method
hvap	89.29	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.989		Crippen Method
mcvol	367.130	ml/mol	McGowan Method
pc	893.20	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	938.42	K	Joback Method
tc	1148.91	K	Joback Method
tf	503.97	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.66	J/mol×K	938.42	Joback Method
cpg	1302.54	J/mol×K	973.50	Joback Method
cpg	1320.70	J/mol×K	1008.58	Joback Method
cpg	1337.18	J/mol×K	1043.67	Joback Method
cpg	1352.01	J/mol×K	1078.75	Joback Method
cpg	1365.24	J/mol×K	1113.83	Joback Method
cpg	1376.89	J/mol×K	1148.91	Joback Method
dvisc	0.0006590	Pa×s	503.97	Joback Method

dvisc	0.0002884	Pa×s	576.38	Joback Method
dvisc	0.0001518	Pa×s	648.79	Joback Method
dvisc	0.0000909	Pa×s	721.19	Joback Method
dvisc	0.0000597	Pa×s	793.60	Joback Method
dvisc	0.0000421	Pa×s	866.01	Joback Method
dvisc	0.0000313	Pa×s	938.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339510&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