1,2-Cyclohexanedicarboxylic acid, 2,5-dimethylphenyl octyl ester

Inchi: InChI=1S/C24H36O4/c1-4-5-6-7-8-11-16-27-23(25)20-12-9-10-13-21(20)24(26)28-22-17

InchiKey: AQVIMIIPNACRHC-UHFFFAOYSA-N

Formula: C24H36O4

SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)ccc1C

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-206.75	kJ/mol	Joback Method
hf	-780.72	kJ/mol	Joback Method
hfus	49.66	kJ/mol	Joback Method
hvap	91.05	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.919		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
pc	1143.66	kPa	Joback Method
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	952.62	K	Joback Method
tc	1172.60	K	Joback Method
tf	559.16	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.33	J/mol×K	952.62	Joback Method
cpg	1135.10	J/mol×K	989.28	Joback Method
cpg	1150.16	J/mol×K	1025.95	Joback Method
cpg	1163.54	J/mol×K	1062.61	Joback Method
cpg	1175.27	J/mol×K	1099.28	Joback Method
cpg	1185.37	J/mol×K	1135.94	Joback Method
cpg	1193.89	J/mol×K	1172.60	Joback Method
dvisc	0.0004299	Pa×s	559.16	Joback Method

dvisc	0.0002396	Pa×s	624.74	Joback Method
dvisc	0.0001492	Pa×s	690.31	Joback Method
dvisc	0.0001009	Pa×s	755.89	Joback Method
dvisc	0.0000726	Pa×s	821.47	Joback Method
dvisc	0.0000549	Pa×s	887.04	Joback Method
dvisc	0.0000431	Pa×s	952.62	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=U339943&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