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

Inchi: InChI=1S/C21H30O4/c1-4-5-8-13-24-20(22)17-9-6-7-10-18(17)21(23)25-19-14-15(2)11-1

InchiKey: BNHPITWQNWDUDG-UHFFFAOYSA-N

Formula: C21H30O4

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

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-232.01	kJ/mol	Joback Method
hf	-718.80	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	84.37	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.749		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	883.98	K	Joback Method
tc	1102.70	K	Joback Method
tf	525.35	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.87	J/mol×K	883.98	Joback Method
cpg	952.99	J/mol×K	920.43	Joback Method
cpg	968.53	J/mol×K	956.89	Joback Method
cpg	982.52	J/mol×K	993.34	Joback Method
cpg	994.96	J/mol×K	1029.79	Joback Method
cpg	1005.88	J/mol×K	1066.24	Joback Method
cpg	1015.31	J/mol×K	1102.70	Joback Method
dvisc	0.0005821	Pa×s	525.35	Joback Method

dvisc	0.0003356	Pa×s	585.12	Joback Method
dvisc	0.0002143	Pa×s	644.89	Joback Method
dvisc	0.0001477	Pa×s	704.66	Joback Method
dvisc	0.0001079	Pa×s	764.44	Joback Method
dvisc	0.0000824	Pa×s	824.21	Joback Method
dvisc	0.0000654	Pa×s	883.98	Joback Method

Sources

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=U339941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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