

1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylphenyl pentyl ester

Inchi:	InChI=1S/C21H30O4/c1-4-5-8-11-24-20(22)18-9-6-7-10-19(18)21(23)25-17-13-15(2)12-
InchiKey:	TXXHXTCGMASHMM-UHFFFAOYSA-N
Formula:	C21H30O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1
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
mvol	287.010	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2504.00		NIST Webbook
rinpol	2504.00		NIST Webbook
tb	883.98	K	Joback Method
tc	1102.70	K	Joback Method
tf	525.35	K	Joback Method
vc	1.083	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.87	J/mol×K	883.98	Joback Method
cpg	1005.88	J/mol×K	1066.24	Joback Method
cpg	994.96	J/mol×K	1029.79	Joback Method
cpg	982.52	J/mol×K	993.34	Joback Method
cpg	968.53	J/mol×K	956.89	Joback Method
cpg	952.99	J/mol×K	920.43	Joback Method
cpg	1015.31	J/mol×K	1102.70	Joback Method
dvisc	0.0000654	Paxs	883.98	Joback Method

dvisc	0.0000824	Paxs	824.21	Joback Method
dvisc	0.0001079	Paxs	764.44	Joback Method
dvisc	0.0001477	Paxs	704.66	Joback Method
dvisc	0.0002143	Paxs	644.89	Joback Method
dvisc	0.0003356	Paxs	585.12	Joback Method
dvisc	0.0005821	Paxs	525.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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