

1,2-Cyclohexanedicarboxylic acid, ethyl 3-methylphenyl ester

Inchi: InChI=1S/C17H22O4/c1-3-20-16(18)14-9-4-5-10-15(14)17(19)21-13-8-6-7-12(2)11-13/h6
InchiKey: LXJCBYZFMXIAAY-UHFFFAOYSA-N
Formula: C17H22O4
SMILES: CCOC(=O)C1CCCCC1C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-256.06	kJ/mol	Joback Method
hf	-624.77	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	74.81	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.270		Crippen Method
mvol	230.650	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	2140.00		NIST Webbook
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tb	787.48	K	Joback Method
tc	1013.74	K	Joback Method
tf	467.75	K	Joback Method
vc	0.860	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.00	J/molxK	787.48	Joback Method
cpg	719.50	J/molxK	825.19	Joback Method
cpg	735.53	J/molxK	862.90	Joback Method
cpg	750.09	J/molxK	900.61	Joback Method
cpg	763.21	J/molxK	938.32	Joback Method
cpg	774.89	J/molxK	976.03	Joback Method
cpg	785.16	J/molxK	1013.74	Joback Method
dvisc	0.0009535	Paxs	467.75	Joback Method

dvisc	0.0005512	Paxs	521.04	Joback Method
dvisc	0.0003528	Paxs	574.33	Joback Method
dvisc	0.0002435	Paxs	627.62	Joback Method
dvisc	0.0001782	Paxs	680.90	Joback Method
dvisc	0.0001364	Paxs	734.19	Joback Method
dvisc	0.0001083	Paxs	787.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339827&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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