

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

Inchi:	InChI=1S/C20H28O4/c1-4-5-10-23-19(21)17-8-6-7-9-18(17)20(22)24-16-12-14(2)11-15(3)
InchiKey:	UHGFTIWGLVXRLE-UHFFFAOYSA-N
Formula:	C20H28O4
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-240.43	kJ/mol	Joback Method
hf	-698.16	kJ/mol	Joback Method
hfus	39.30	kJ/mol	Joback Method
hvap	82.15	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.359		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2412.00		NIST Webbook
tb	861.10	K	Joback Method
tc	1080.91	K	Joback Method
tf	514.08	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.16	J/molxK	861.10	Joback Method
cpg	893.38	J/molxK	897.74	Joback Method
cpg	909.05	J/molxK	934.37	Joback Method
cpg	923.19	J/molxK	971.01	Joback Method
cpg	935.82	J/molxK	1007.64	Joback Method
cpg	946.96	J/molxK	1044.28	Joback Method
cpg	956.61	J/molxK	1080.91	Joback Method
dvisc	0.0006387	Paxs	514.08	Joback Method
dvisc	0.0003727	Paxs	571.92	Joback Method

dvisc	0.0002401	Paxs	629.75	Joback Method
dvisc	0.0001666	Paxs	687.59	Joback Method
dvisc	0.0001223	Paxs	745.43	Joback Method
dvisc	0.0000939	Paxs	803.26	Joback Method
dvisc	0.0000747	Paxs	861.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339614&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
mvol:	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

Latest version available from:

<https://www.chemeo.com/cid/87-457-9/1-2-Cyclohexanedicarboxylic-acid-butyl-3-5-dimethylphenyl-ester.pdf>

Generated by Cheméo on 2024-04-26 08:40:44.263071323 +0000 UTC m=+16410093.183648639.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.