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

Inchi: InChI=1S/C20H28O4/c1-4-5-12-23-19(21)16-8-6-7-9-17(16)20(22)24-18-13-14(2)10-11-1

InchiKey: ITNWHOJPWLAFLF-UHFFFAOYSA-N

Formula: C20H28O4

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

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	2393.00		NIST Webbook
rinpol	2393.00		NIST Webbook
tb	861.10	K	Joback Method
tc	1080.91	K	Joback Method
tf	514.08	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.16	J/mol×K	861.10	Joback Method
cpg	946.96	J/mol×K	1044.28	Joback Method
cpg	935.82	J/mol×K	1007.64	Joback Method
cpg	923.19	J/mol×K	971.01	Joback Method
cpg	909.05	J/mol×K	934.37	Joback Method
cpg	893.38	J/mol×K	897.74	Joback Method
cpg	956.61	J/mol×K	1080.91	Joback Method
dvisc	0.0000747	Pa×s	861.10	Joback Method

dvisc	0.0000939	Pa×s	803.26	Joback Method
dvisc	0.0001223	Pa×s	745.43	Joback Method
dvisc	0.0001666	Pa×s	687.59	Joback Method
dvisc	0.0002401	Pa×s	629.75	Joback Method
dvisc	0.0003727	Pa×s	571.92	Joback Method
dvisc	0.0006387	Pa×s	514.08	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U339940&Units=SI
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

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