cis-Cyclohex-4-en-1,2-dicarboxylic acid, butyl phenethyl ester

Inchi: InChI=1S/C20H26O4/c1-2-3-14-23-19(21)17-11-7-8-12-18(17)20(22)24-15-13-16-9-5-4-6

InchiKey: ANYOCAQEWQNMSP-UHFFFAOYSA-N

Formula: C20H26O4

SMILES: CCCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-191.21	kJ/mol	Joback Method
hf	-617.44	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	81.11	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.698		Crippen Method
mcvol	268.620	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2409.00		NIST Webbook
rinpol	2409.00		NIST Webbook
tb	850.30	K	Joback Method
tc	1069.77	K	Joback Method
tf	489.80	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.95	J/mol×K	850.30	Joback Method
cpg	917.98	J/mol×K	1033.19	Joback Method
cpg	907.02	J/mol×K	996.61	Joback Method
cpg	894.67	J/mol×K	960.04	Joback Method
cpg	880.90	J/mol×K	923.46	Joback Method
cpg	865.67	J/mol×K	886.88	Joback Method
cpg	927.59	J/mol×K	1069.77	Joback Method
dvisc	0.0000782	Pa×s	850.30	Joback Method

dvisc	0.0001000	Pa×s	790.22	Joback Method
dvisc	0.0001330	Pa×s	730.13	Joback Method
dvisc	0.0001864	Pa×s	670.05	Joback Method
dvisc	0.0002790	Pa×s	609.97	Joback Method
dvisc	0.0004562	Pa×s	549.88	Joback Method
dvisc	0.0008414	Pa×s	489.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382790&Units=SI

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