cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(2-methylbutyl) ester

Inchi: InChI=1S/C18H30O4/c1-5-13(3)11-21-17(19)15-9-7-8-10-16(15)18(20)22-12-14(4)6-2/h7
InchiKey: DZWIAYAUFVOENZ-UHFFFAOYSA-N
Formula: C18H30O4
SMILES: CCC(C)COC(=O)C1CC=CCC1C(=O)OCC(C)CC
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-325.34	kJ/mol	Joback Method
hf	-823.25	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.747		Crippen Method
mcvol	264.200	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	776.98	K	Joback Method
tc	977.20	K	Joback Method
tf	410.84	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.15	J/mol×K	776.98	Joback Method
cpg	841.87	J/mol×K	810.35	Joback Method
cpg	859.31	J/mol×K	843.72	Joback Method
cpg	875.50	J/mol×K	877.09	Joback Method
cpg	890.44	J/mol×K	910.46	Joback Method
cpg	904.16	J/mol×K	943.83	Joback Method
cpg	916.66	J/mol×K	977.20	Joback Method
dvisc	0.0016490	Pa×s	410.84	Joback Method

dvisc	0.0007278	Pa×s	471.86	Joback Method
dvisc	0.0003874	Pa×s	532.89	Joback Method
dvisc	0.0002347	Pa×s	593.91	Joback Method
dvisc	0.0001561	Pa×s	654.93	Joback Method
dvisc	0.0001113	Pa×s	715.96	Joback Method
dvisc	0.0000837	Pa×s	776.98	Joback Method

Sources

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=U382697&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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