

cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(3-methylbutyl) ester

Inchi:	InChI=1S/C18H30O4/c1-13(2)9-11-21-17(19)15-7-5-6-8-16(15)18(20)22-12-10-14(3)4/h5
InchiKey:	YUDDZCVBEWFWDE-UHFFFAOYSA-N
Formula:	C18H30O4
SMILES:	CC(C)CCOC(=O)C1CC=CCC1C(=O)OCCC(C)C
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	2012.00		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/molxK	776.98	Joback Method
cpg	904.16	J/molxK	943.83	Joback Method
cpg	890.44	J/molxK	910.46	Joback Method
cpg	875.50	J/molxK	877.09	Joback Method
cpg	859.31	J/molxK	843.72	Joback Method
cpg	841.87	J/molxK	810.35	Joback Method
cpg	916.66	J/molxK	977.20	Joback Method
dvisc	0.0000837	Paxs	776.98	Joback Method
dvisc	0.0001113	Paxs	715.96	Joback Method

dvisc	0.0001561	Paxs	654.93	Joback Method
dvisc	0.0002347	Paxs	593.91	Joback Method
dvisc	0.0003874	Paxs	532.89	Joback Method
dvisc	0.0007278	Paxs	471.86	Joback Method
dvisc	0.0016490	Paxs	410.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382771&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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