

cis-Cyclohex-4-en-1,2-dicarboxylic acid, hexyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C20H34O4/c1-5-7-8-11-14-23-19(21)16-12-9-10-13-17(16)20(22)24-18(6-2)15
InchiKey:	RFZKOYQLSBPIEQ-UHFFFAOYSA-N
Formula:	C20H34O4
SMILES:	CCCCCOC(=O)C1CC=CCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	338.48

Physical Properties

Property code	Value	Unit	Source
gf	-308.50	kJ/mol	Joback Method
hf	-864.53	kJ/mol	Joback Method
hfus	40.21	kJ/mol	Joback Method
hvap	78.06	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.670		Crippen Method
mvol	292.380	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2237.00		NIST Webbook
rinpol	2237.00		NIST Webbook
tb	822.74	K	Joback Method
tc	1022.27	K	Joback Method
tf	433.38	K	Joback Method
vc	1.109	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.60	J/molxK	822.74	Joback Method
cpg	961.44	J/molxK	856.00	Joback Method
cpg	978.93	J/molxK	889.25	Joback Method
cpg	995.09	J/molxK	922.51	Joback Method
cpg	1009.94	J/molxK	955.76	Joback Method
cpg	1023.50	J/molxK	989.02	Joback Method
cpg	1035.78	J/molxK	1022.27	Joback Method
dvisc	0.0013422	Paxs	433.38	Joback Method

dvisc	0.0005809	Paxs	498.27	Joback Method
dvisc	0.0003050	Paxs	563.17	Joback Method
dvisc	0.0001829	Paxs	628.06	Joback Method
dvisc	0.0001207	Paxs	692.95	Joback Method
dvisc	0.0000855	Paxs	757.85	Joback Method
dvisc	0.0000640	Paxs	822.74	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=U382763&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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