

1,2-Cyclohexanedicarboxylic acid, heptyl 3-methylbut-2-yl ester

Inchi:	InChI=1S/C20H36O4/c1-5-6-7-8-11-14-23-19(21)17-12-9-10-13-18(17)20(22)24-16(4)15
InchiKey:	CZVBDGRFMYFANT-UHFFFAOYSA-N
Formula:	C20H36O4
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)OC(C)C(C)C
Mol. weight [g/mol]:	340.50

Physical Properties

Property code	Value	Unit	Source
gf	-338.46	kJ/mol	Joback Method
hf	-922.31	kJ/mol	Joback Method
hfus	38.99	kJ/mol	Joback Method
hvap	77.77	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.894		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinsol	2223.00		NIST Webbook
tb	823.58	K	Joback Method
tc	1022.33	K	Joback Method
tf	432.62	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.46	J/molxK	823.58	Joback Method
cpg	990.04	J/molxK	856.70	Joback Method
cpg	1008.24	J/molxK	889.83	Joback Method
cpg	1025.07	J/molxK	922.95	Joback Method
cpg	1040.54	J/molxK	956.08	Joback Method
cpg	1054.67	J/molxK	989.20	Joback Method
cpg	1067.49	J/molxK	1022.33	Joback Method
dvisc	0.0014062	Paxs	432.62	Joback Method
dvisc	0.0005879	Paxs	497.78	Joback Method

dvisc	0.0003007	Paxs	562.94	Joback Method
dvisc	0.0001768	Paxs	628.10	Joback Method
dvisc	0.0001149	Paxs	693.26	Joback Method
dvisc	0.0000804	Paxs	758.42	Joback Method
dvisc	0.0000595	Paxs	823.58	Joback Method

Sources

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=U339560&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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