

1,2-Cyclohexanedicarboxylic acid, isobutyl isoheptyl ester

Inchi:	InChI=1S/C18H32O4/c1-13(2)8-7-11-21-17(19)15-9-5-6-10-16(15)18(20)22-12-14(3)4/h1
InchiKey:	ANEWXIISWUKCHF-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	CC(C)CCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-355.30	kJ/mol	Joback Method
hf	-881.03	kJ/mol	Joback Method
hfus	33.81	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.971		Crippen Method
mvol	268.500	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	777.82	K	Joback Method
tc	976.97	K	Joback Method
tf	410.08	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.75	J/molxK	777.82	Joback Method
cpg	869.25	J/molxK	811.01	Joback Method
cpg	887.45	J/molxK	844.20	Joback Method
cpg	904.36	J/molxK	877.39	Joback Method
cpg	919.99	J/molxK	910.59	Joback Method
cpg	934.35	J/molxK	943.78	Joback Method
cpg	947.45	J/molxK	976.97	Joback Method
dvisc	0.0017505	Paxs	410.08	Joback Method

dvisc	0.0007450	Paxs	471.37	Joback Method
dvisc	0.0003860	Paxs	532.66	Joback Method
dvisc	0.0002290	Paxs	593.95	Joback Method
dvisc	0.0001498	Paxs	655.24	Joback Method
dvisc	0.0001054	Paxs	716.53	Joback Method
dvisc	0.0000784	Paxs	777.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339426&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

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