

1,2-Cyclohexanedicarboxylic acid, isoheptyl 4-octyl ester

Inchi:	InChI=1S/C22H40O4/c1-5-7-13-18(11-6-2)26-22(24)20-15-9-8-14-19(20)21(23)25-16-10
InchiKey:	YDAYAWZSMYTDGX-UHFFFAOYSA-N
Formula:	C22H40O4
SMILES:	CCCCC(CCC)OC(=O)C1CCCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	368.55

Physical Properties

Property code	Value	Unit	Source
gf	-321.62	kJ/mol	Joback Method
hf	-963.59	kJ/mol	Joback Method
hfus	44.17	kJ/mol	Joback Method
hvap	82.22	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.674		Crippen Method
mvol	324.860	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	869.34	K	Joback Method
tc	1070.39	K	Joback Method
tf	455.16	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.91	J/molxK	869.34	Joback Method
cpg	1113.57	J/molxK	902.85	Joback Method
cpg	1131.72	J/molxK	936.36	Joback Method
cpg	1148.41	J/molxK	969.87	Joback Method
cpg	1163.65	J/molxK	1003.38	Joback Method
cpg	1177.46	J/molxK	1036.88	Joback Method
cpg	1189.87	J/molxK	1070.39	Joback Method
dvisc	0.0011117	Paxs	455.16	Joback Method

dvisc	0.0004572	Paxs	524.19	Joback Method
dvisc	0.0002313	Paxs	593.22	Joback Method
dvisc	0.0001348	Paxs	662.25	Joback Method
dvisc	0.0000870	Paxs	731.28	Joback Method
dvisc	0.0000606	Paxs	800.31	Joback Method
dvisc	0.0000447	Paxs	869.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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