

cis-Cyclohex-4-en-1,2-dicarboxylic acid, isoheptyl phenethyl ester

Inchi:	InChI=1S/C22H30O4/c1-17(2)9-8-15-25-21(23)19-12-6-7-13-20(19)22(24)26-16-14-18-1
InchiKey:	ZRYNUTOQDUMPTO-UHFFFAOYSA-N
Formula:	C22H30O4
SMILES:	CC(C)CCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	358.47

Physical Properties

Property code	Value	Unit	Source
gf	-176.81	kJ/mol	Joback Method
hf	-664.00	kJ/mol	Joback Method
hfus	42.96	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.334		Crippen Method
mcvol	296.800	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2568.00		NIST Webbook
tb	895.62	K	Joback Method
tc	1115.41	K	Joback Method
tf	497.34	K	Joback Method
vc	1.119	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.31	J/molxK	895.62	Joback Method
cpg	1036.51	J/molxK	1078.78	Joback Method
cpg	1025.87	J/molxK	1042.15	Joback Method
cpg	1013.77	J/molxK	1005.51	Joback Method
cpg	1000.16	J/molxK	968.88	Joback Method
cpg	985.03	J/molxK	932.25	Joback Method
cpg	1045.74	J/molxK	1115.41	Joback Method
dvisc	0.0000545	Paxs	895.62	Joback Method
dvisc	0.0000711	Paxs	829.24	Joback Method

dvisc	0.0000971	Paxs	762.86	Joback Method
dvisc	0.0001407	Paxs	696.48	Joback Method
dvisc	0.0002205	Paxs	630.10	Joback Method
dvisc	0.0003841	Paxs	563.72	Joback Method
dvisc	0.0007761	Paxs	497.34	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=U382792&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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