

cis-Cyclohex-4-en-1,2-dicarboxylic acid, 2-ethylbutyl heptyl ester

Inchi:	InChI=1S/C21H36O4/c1-4-7-8-9-12-15-24-20(22)18-13-10-11-14-19(18)21(23)25-16-17(
InchiKey:	ACSZNUBOFHDJQG-UHFFFAOYSA-N
Formula:	C21H36O4
SMILES:	CCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC
Mol. weight [g/mol]:	352.51

Physical Properties

Property code	Value	Unit	Source
gf	-297.64	kJ/mol	Joback Method
hf	-879.89	kJ/mol	Joback Method
hfus	46.32	kJ/mol	Joback Method
hvap	80.68	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.062		Crippen Method
mvol	306.470	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	2337.00		NIST Webbook
rinpol	2337.00		NIST Webbook
tb	846.06	K	Joback Method
tc	1044.69	K	Joback Method
tf	459.65	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.95	J/molxK	846.06	Joback Method
cpg	1021.70	J/molxK	879.16	Joback Method
cpg	1039.10	J/molxK	912.27	Joback Method
cpg	1055.15	J/molxK	945.37	Joback Method
cpg	1069.87	J/molxK	978.48	Joback Method
cpg	1083.30	J/molxK	1011.58	Joback Method
cpg	1095.45	J/molxK	1044.69	Joback Method
dvisc	0.0010253	Paxs	459.65	Joback Method

dvisc	0.0004795	Paxs	524.05	Joback Method
dvisc	0.0002648	Paxs	588.45	Joback Method
dvisc	0.0001644	Paxs	652.86	Joback Method
dvisc	0.0001112	Paxs	717.26	Joback Method
dvisc	0.0000802	Paxs	781.66	Joback Method
dvisc	0.0000608	Paxs	846.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382809&Units=SI
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

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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