

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

Inchi:	InChI=1S/C25H44O4/c1-3-5-7-9-10-11-13-17-21-29-25(27)23-19-15-14-18-22(23)24(26)
InchiKey:	QMZZLEOWGUEGEZ-UHFFFAOYSA-N
Formula:	C25H44O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCCC
Mol. weight [g/mol]:	408.61

Physical Properties

Property code	Value	Unit	Source
gf	-261.52	kJ/mol	Joback Method
hf	-957.17	kJ/mol	Joback Method
hfus	60.21	kJ/mol	Joback Method
hvap	89.97	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.766		Crippen Method
mvol	362.830	ml/mol	McGowan Method
pc	908.34	kPa	Joback Method
rinpol	2781.00		NIST Webbook
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tb	938.02	K	Joback Method
tc	1148.40	K	Joback Method
tf	519.73	K	Joback Method
vc	1.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.69	J/molxK	938.02	Joback Method
cpg	1270.92	J/molxK	973.08	Joback Method
cpg	1288.52	J/molxK	1008.15	Joback Method
cpg	1304.50	J/molxK	1043.21	Joback Method
cpg	1318.92	J/molxK	1078.27	Joback Method
cpg	1331.81	J/molxK	1113.34	Joback Method
cpg	1343.20	J/molxK	1148.40	Joback Method
dvisc	0.0005756	Paxs	519.73	Joback Method

dvisc	0.0002790	Paxs	589.45	Joback Method
dvisc	0.0001577	Paxs	659.16	Joback Method
dvisc	0.0000994	Paxs	728.88	Joback Method
dvisc	0.0000679	Paxs	798.59	Joback Method
dvisc	0.0000493	Paxs	868.31	Joback Method
dvisc	0.0000375	Paxs	938.02	Joback Method

Sources

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=U382676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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