

Bis(2-ethylhexyl) 4-cyclohexene-1,2-dicarboxylate

Other names: 4-Cyclohexene-1,2-dicarboxylic acid, di(2-ethylhexyl) ester

Inchi: InChI=1S/C24H42O4/c1-5-9-13-19(7-3)17-27-23(25)21-15-11-12-16-22(21)24(26)28-18-

InchiKey: SVVBLKNHJWTATO-UHFFFAOYSA-N

Formula: C24H42O4

SMILES: CCCCC(CC)COC(=O)C1CC=CCC1C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 394.59

CAS: 2915-49-3

Physical Properties

Property code	Value	Unit	Source
gf	-274.82	kJ/mol	Joback Method
hf	-947.09	kJ/mol	Joback Method
hfus	50.57	kJ/mol	Joback Method
hvap	86.97	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.088		Crippen Method
mcvol	348.740	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
tb	914.26	K	Joback Method
tc	1120.89	K	Joback Method
tf	478.46	K	Joback Method
vc	1.333	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.48	J/mol×K	914.26	Joback Method
cpg	1208.56	J/mol×K	948.70	Joback Method
cpg	1226.06	J/mol×K	983.14	Joback Method
cpg	1242.01	J/mol×K	1017.57	Joback Method
cpg	1256.43	J/mol×K	1052.01	Joback Method
cpg	1269.37	J/mol×K	1086.45	Joback Method
cpg	1280.86	J/mol×K	1120.89	Joback Method
dvisc	0.0008462	Paxs	478.46	Joback Method

dvisc	0.0003540	Paxs	551.09	Joback Method
dvisc	0.0001815	Paxs	623.73	Joback Method
dvisc	0.0001069	Paxs	696.36	Joback Method
dvisc	0.0000696	Paxs	768.99	Joback Method
dvisc	0.0000488	Paxs	841.63	Joback Method
dvisc	0.0000362	Paxs	914.26	Joback Method

Sources

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=C2915493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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