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

Inchi: InChI=1S/C19H32O4/c1-4-7-10-13-22-18(20)16-11-8-9-12-17(16)19(21)23-14-15(5-2)6-3

InchiKey: YGKJHVJIIMXDCE-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-314.48	kJ/mol	Joback Method
hf	-838.61	kJ/mol	Joback Method
hfus	41.14	kJ/mol	Joback Method
hvap	76.22	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.282		Crippen Method
mcvol	278.290	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	800.30	K	Joback Method
tc	997.70	K	Joback Method
tf	437.11	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.99	J/mol×K	800.30	Joback Method
cpg	962.35	J/mol×K	964.80	Joback Method
cpg	948.76	J/mol×K	931.90	Joback Method
cpg	933.94	J/mol×K	899.00	Joback Method
cpg	917.88	J/mol×K	866.10	Joback Method
cpg	900.57	J/mol×K	833.20	Joback Method
cpg	974.75	J/mol×K	997.70	Joback Method
dvisc	0.0000798	Pa×s	800.30	Joback Method

dvisc	0.0001047	Pa×s	739.77	Joback Method
dvisc	0.0001442	Pa×s	679.24	Joback Method
dvisc	0.0002113	Pa×s	618.71	Joback Method
dvisc	0.0003365	Pa×s	558.17	Joback Method
dvisc	0.0006002	Pa×s	497.64	Joback Method
dvisc	0.0012563	Pa×s	437.11	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=U382807&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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