Isophthalic acid, 2-cyclohexylethyl undecyl ester

Inchi: InChI=1S/C27H42O4/c1-2-3-4-5-6-7-8-9-13-20-30-26(28)24-17-14-18-25(22-24)27(29)31

InchiKey: PGGGZFKYIKYTLA-UHFFFAOYSA-N

Formula: C27H42O4

SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC2CCCCC2)c1

Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-164.15	kJ/mol	Joback Method
hf	-810.83	kJ/mol	Joback Method
hfus	56.75	kJ/mol	Joback Method
hvap	97.38	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	7.501		Crippen Method
mcvol	371.550	ml/mol	McGowan Method
pc	978.40	kPa	Joback Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook
tb	1020.95	K	Joback Method
tc	1250.04	K	Joback Method
tf	584.69	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.74	J/mol×K	1020.95	Joback Method
cpg	1366.42	J/mol×K	1211.86	Joback Method
cpg	1356.63	J/mol×K	1173.67	Joback Method
cpg	1345.24	J/mol×K	1135.49	Joback Method
cpg	1332.17	J/mol×K	1097.31	Joback Method
cpg	1317.35	J/mol×K	1059.13	Joback Method
cpg	1374.66	J/mol×K	1250.04	Joback Method
dvisc	0.0000200	Pa×s	1020.95	Joback Method

dvisc	0.0000264	Pa×s	948.24	Joback Method
dvisc	0.0000365	Pa×s	875.53	Joback Method
dvisc	0.0000535	Pa×s	802.82	Joback Method
dvisc	0.0000847	Pa×s	730.11	Joback Method
dvisc	0.0001482	Pa×s	657.40	Joback Method
dvisc	0.0002982	Pa×s	584.69	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=U343816&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