Isophthalic acid, di(2-cyclohexylethyl) ester

Inchi: InChI=1S/C24H34O4/c25-23(27-16-14-19-8-3-1-4-9-19)21-12-7-13-22(18-21)24(26)28-1
InchiKey: ZOLLWCITYOPDLK-UHFFFAOYSA-N
Formula: C24H34O4
SMILES: O=C(OCCC1CCCCC1)c1cccc(C(=O)OCCC2CCCCC2)c1
Mol. weight [g/mol]: 386.52

Physical Properties

Property code	Value	Unit	Source
gf	-164.96	kJ/mol	Joback Method
hf	-694.59	kJ/mol	Joback Method
hfus	40.81	kJ/mol	Joback Method
hvap	91.13	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	5.941		Crippen Method
mcvol	318.420	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	3222.00		NIST Webbook
rinpol	3222.00		NIST Webbook
tb	971.86	K	Joback Method
tc	1208.22	K	Joback Method
tf	558.26	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.09	J/mol×K	971.86	Joback Method
cpg	1125.66	J/mol×K	1011.25	Joback Method
cpg	1140.24	J/mol×K	1050.65	Joback Method
cpg	1152.88	J/mol×K	1090.04	Joback Method
cpg	1163.64	J/mol×K	1129.43	Joback Method
cpg	1172.60	J/mol×K	1168.83	Joback Method
cpg	1179.79	J/mol×K	1208.22	Joback Method
dvisc	0.0004818	Pa×s	558.26	Joback Method

dvisc	0.0002401	Pa×s	627.19	Joback Method
dvisc	0.0001373	Pa×s	696.13	Joback Method
dvisc	0.0000869	Pa×s	765.06	Joback Method
dvisc	0.0000593	Pa×s	833.99	Joback Method
dvisc	0.0000429	Pa×s	902.93	Joback Method
dvisc	0.0000325	Pa×s	971.86	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=U343817&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