Isophthalic acid, cyclohexylmethyl nonyl ester

Inchi: InChI=1S/C24H36O4/c1-2-3-4-5-6-7-11-17-27-23(25)21-15-12-16-22(18-21)24(26)28-19
InchiKey: FSDYGECMQKESJK-UHFFFAOYSA-N
Formula: C24H36O4
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-189.41	kJ/mol	Joback Method
hf	-748.91	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	90.70	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.331		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	952.31	K	Joback Method
tc	1171.98	K	Joback Method
tf	550.88	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1114.62	J/mol×K	952.31	Joback Method
cpg	1182.47	J/mol×K	1135.36	Joback Method
cpg	1171.94	J/mol×K	1098.75	Joback Method
cpg	1159.94	J/mol×K	1062.14	Joback Method
cpg	1146.42	J/mol×K	1025.53	Joback Method
cpg	1131.32	J/mol×K	988.92	Joback Method
cpg	1191.57	J/mol×K	1171.98	Joback Method
dvisc	0.0000317	Pa×s	952.31	Joback Method

dvisc	0.0000415	Pa×s	885.40	Joback Method
dvisc	0.0000569	Pa×s	818.50	Joback Method
dvisc	0.0000825	Pa×s	751.60	Joback Method
dvisc	0.0001285	Pa×s	684.69	Joback Method
dvisc	0.0002205	Pa×s	617.78	Joback Method
dvisc	0.0004314	Pa×s	550.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U343831&Units=SI

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