Phthalic acid, di(cycloheptyl) ester

Other names: Dicycloheptyl phthalate
Inchi: InChI=1S/C22H30O4/c23-21(25-17-11-5-1-2-6-12-17)19-15-9-10-16-20(19)22(24)26-18-
InchiKey: GULQIIBSEHFYOM-UHFFFAOYSA-N
Formula: C22H30O4
SMILES: O=C(OC1CCCCCC1)c1ccccc1C(=O)OC1CCCCCC1
Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-206.00	kJ/mol	Joback Method
hf	-665.63	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	87.02	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.446		Crippen Method
mcvol	290.240	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2735.00		NIST Webbook
tb	934.64	K	Joback Method
tc	1184.76	K	Joback Method
tf	528.68	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.44	J/mol×K	934.64	Joback Method
cpg	1057.94	J/mol×K	1143.08	Joback Method
cpg	1050.19	J/mol×K	1101.39	Joback Method
cpg	1040.10	J/mol×K	1059.70	Joback Method
cpg	1027.64	J/mol×K	1018.01	Joback Method
cpg	1012.76	J/mol×K	976.33	Joback Method
cpg	1063.39	J/mol×K	1184.76	Joback Method
dvisc	0.0000202	Pa×s	934.64	Joback Method

dvisc	0.0000277	Pa×s	866.98	Joback Method
dvisc	0.0000400	Pa×s	799.32	Joback Method
dvisc	0.0000619	Pa×s	731.66	Joback Method
dvisc	0.0001048	Pa×s	664.00	Joback Method
dvisc	0.0001998	Pa×s	596.34	Joback Method
dvisc	0.0004493	Pa×s	528.68	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=U322837&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