

1,2-Cyclohexanedicarboxylic acid, 2-biphenyl hexyl ester

Inchi:	InChI=1S/C26H32O4/c1-2-3-4-12-19-29-25(27)22-16-8-9-17-23(22)26(28)30-24-18-11-1
InchiKey:	RIFPUXXXQVKNID-UHFFFAOYSA-N
Formula:	C26H32O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	408.53

Physical Properties

Property code	Value	Unit	Source
gf	-67.87	kJ/mol	Joback Method
hf	-574.00	kJ/mol	Joback Method
hfus	49.27	kJ/mol	Joback Method
hvap	97.12	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.189		Crippen Method
mcvol	333.700	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	2977.00		NIST Webbook
tb	1020.08	K	Joback Method
tc	1259.54	K	Joback Method
tf	595.60	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1135.15	J/molxK	1020.08	Joback Method
cpg	1149.15	J/molxK	1059.99	Joback Method
cpg	1161.29	J/molxK	1099.90	Joback Method
cpg	1171.63	J/molxK	1139.81	Joback Method
cpg	1180.23	J/molxK	1179.72	Joback Method
cpg	1187.18	J/molxK	1219.63	Joback Method
cpg	1192.53	J/molxK	1259.54	Joback Method
dvisc	0.0003491	Paxs	595.60	Joback Method
dvisc	0.0001909	Paxs	666.35	Joback Method

dvisc	0.0001172	Paxs	737.09	Joback Method
dvisc	0.0000783	Paxs	807.84	Joback Method
dvisc	0.0000559	Paxs	878.59	Joback Method
dvisc	0.0000419	Paxs	949.33	Joback Method
dvisc	0.0000327	Paxs	1020.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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