

Isophthalic acid, butyl 4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C22H32O4/c1-5-6-14-25-20(23)16-8-7-9-17(15-16)21(24)26-19-12-10-18(11-1
InchiKey:	PICCGQREHDKOIT-UHFFFAOYSA-N
Formula:	C22H32O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1
Mol. weight [g/mol]:	360.49

Physical Properties

Property code	Value	Unit	Source
gf	-211.12	kJ/mol	Joback Method
hf	-736.72	kJ/mol	Joback Method
hfus	37.45	kJ/mol	Joback Method
hvap	84.64	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.405		Crippen Method
mvol	301.100	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2713.00		NIST Webbook
rinpol	2713.00		NIST Webbook
tb	898.65	K	Joback Method
tc	1122.47	K	Joback Method
tf	526.52	K	Joback Method
vc	1.129	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.26	J/molxK	898.65	Joback Method
cpg	1069.07	J/molxK	1085.17	Joback Method
cpg	1057.70	J/molxK	1047.86	Joback Method
cpg	1044.90	J/molxK	1010.56	Joback Method
cpg	1030.59	J/molxK	973.26	Joback Method
cpg	1014.73	J/molxK	935.95	Joback Method
cpg	1079.04	J/molxK	1122.47	Joback Method
dvisc	0.0000434	Paxs	898.65	Joback Method

dvisc	0.0000566	Paxs	836.63	Joback Method
dvisc	0.0000769	Paxs	774.61	Joback Method
dvisc	0.0001105	Paxs	712.59	Joback Method
dvisc	0.0001699	Paxs	650.56	Joback Method
dvisc	0.0002861	Paxs	588.54	Joback Method
dvisc	0.0005448	Paxs	526.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345735&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

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