

Isophthalic acid, heptyl 4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C25H38O4/c1-5-6-7-8-9-17-28-23(26)19-11-10-12-20(18-19)24(27)29-22-15-1
InchiKey:	OBHHQKJWHXWKBL-UHFFFAOYSA-N
Formula:	C25H38O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1
Mol. weight [g/mol]:	402.57

Physical Properties

Property code	Value	Unit	Source
gf	-185.86	kJ/mol	Joback Method
hf	-798.64	kJ/mol	Joback Method
hfus	45.22	kJ/mol	Joback Method
hvap	91.32	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.575		Crippen Method
mvol	343.370	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	3026.00		NIST Webbook
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tb	967.29	K	Joback Method
tc	1191.51	K	Joback Method
tf	560.33	K	Joback Method
vc	1.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.72	J/molxK	967.29	Joback Method
cpg	1197.81	J/molxK	1004.66	Joback Method
cpg	1213.24	J/molxK	1042.03	Joback Method
cpg	1227.06	J/molxK	1079.40	Joback Method
cpg	1239.34	J/molxK	1116.77	Joback Method
cpg	1250.15	J/molxK	1154.14	Joback Method
cpg	1259.56	J/molxK	1191.51	Joback Method
dvisc	0.0003835	Paxs	560.33	Joback Method

dvisc	0.0001953	Paxs	628.16	Joback Method
dvisc	0.0001135	Paxs	695.98	Joback Method
dvisc	0.0000726	Paxs	763.81	Joback Method
dvisc	0.0000500	Paxs	831.64	Joback Method
dvisc	0.0000364	Paxs	899.46	Joback Method
dvisc	0.0000277	Paxs	967.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345739&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
mccvol:	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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