

Isophthalic acid, 3,3-dimethylbut-2-yl heptyl ester

Inchi:	InChI=1S/C21H32O4/c1-6-7-8-9-10-14-24-19(22)17-12-11-13-18(15-17)20(23)25-16(2)2
InchiKey:	KMCRYCSSYSUMGJ-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)(C)C)c1
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-238.72	kJ/mol	Joback Method
hf	-755.34	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	81.91	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.405		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinsol	2393.00		NIST Webbook
tb	860.45	K	Joback Method
tc	1067.71	K	Joback Method
tf	497.11	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.43	J/molxK	860.45	Joback Method
cpg	955.02	J/molxK	894.99	Joback Method
cpg	970.40	J/molxK	929.54	Joback Method
cpg	984.62	J/molxK	964.08	Joback Method
cpg	997.72	J/molxK	998.62	Joback Method
cpg	1009.74	J/molxK	1033.16	Joback Method
cpg	1020.73	J/molxK	1067.71	Joback Method
dvisc	0.0005578	Paxs	497.11	Joback Method
dvisc	0.0002722	Paxs	557.67	Joback Method

dvisc	0.0001529	Paxs	618.22	Joback Method
dvisc	0.0000952	Paxs	678.78	Joback Method
dvisc	0.0000640	Paxs	739.34	Joback Method
dvisc	0.0000457	Paxs	799.89	Joback Method
dvisc	0.0000343	Paxs	860.45	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=U356552&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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