

Isophthalic acid, butyl 2,5-dimethylphenyl ester

Inchi:	InChI=1S/C20H22O4/c1-4-5-11-23-19(21)16-7-6-8-17(13-16)20(22)24-18-12-14(2)9-10-
InchiKey:	GYULITVZPLDCKZ-UHFFFAOYSA-N
Formula:	C20H22O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2cc(C)ccc2C)c1
Mol. weight [g/mol]:	326.39

Physical Properties

Property code	Value	Unit	Source
gf	-154.39	kJ/mol	Joback Method
hf	-507.08	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	84.96	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.480		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2638.00		NIST Webbook
tb	877.88	K	Joback Method
tc	1103.17	K	Joback Method
tf	549.88	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.21	J/molxK	877.88	Joback Method
cpg	793.20	J/molxK	915.43	Joback Method
cpg	805.90	J/molxK	952.98	Joback Method
cpg	817.33	J/molxK	990.52	Joback Method
cpg	827.51	J/molxK	1028.07	Joback Method
cpg	836.47	J/molxK	1065.62	Joback Method
cpg	844.23	J/molxK	1103.17	Joback Method
dvisc	0.0004003	Paxs	549.88	Joback Method
dvisc	0.0002508	Paxs	604.55	Joback Method

dvisc	0.0001698	Paxs	659.21	Joback Method
dvisc	0.0001221	Paxs	713.88	Joback Method
dvisc	0.0000919	Paxs	768.55	Joback Method
dvisc	0.0000719	Paxs	823.21	Joback Method
dvisc	0.0000580	Paxs	877.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344540&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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