

Isophthalic acid, heptyl 3-methylbutyl ester

Inchi:	InChI=1S/C20H30O4/c1-4-5-6-7-8-13-23-19(21)17-10-9-11-18(15-17)20(22)24-14-12-16
InchiKey:	HLOWJJPDLVFEFX-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)c1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-249.98	kJ/mol	Joback Method
hf	-725.95	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	80.98	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.017		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1349.66	kPa	Joback Method
rinpol	2417.00		NIST Webbook
tb	840.80	K	Joback Method
tc	1042.55	K	Joback Method
tf	483.42	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.24	J/molxK	840.80	Joback Method
cpg	894.49	J/molxK	874.43	Joback Method
cpg	909.59	J/molxK	908.05	Joback Method
cpg	923.56	J/molxK	941.68	Joback Method
cpg	936.41	J/molxK	975.30	Joback Method
cpg	948.18	J/molxK	1008.93	Joback Method
cpg	958.87	J/molxK	1042.55	Joback Method
dvisc	0.0006723	Paxs	483.42	Joback Method
dvisc	0.0003442	Paxs	542.98	Joback Method

dvisc	0.0002012	Paxs	602.55	Joback Method
dvisc	0.0001295	Paxs	662.11	Joback Method
dvisc	0.0000897	Paxs	721.67	Joback Method
dvisc	0.0000656	Paxs	781.24	Joback Method
dvisc	0.0000502	Paxs	840.80	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=U356462&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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