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/mol×K	840.80	Joback Method
cpg	948.18	J/mol×K	1008.93	Joback Method
cpg	936.41	J/mol×K	975.30	Joback Method
cpg	923.56	J/mol×K	941.68	Joback Method
cpg	909.59	J/mol×K	908.05	Joback Method
cpg	894.49	J/mol×K	874.43	Joback Method
cpg	958.87	J/mol×K	1042.55	Joback Method
dvisc	0.0000502	Pa×s	840.80	Joback Method
dvisc	0.0000656	Pa×s	781.24	Joback Method

dvisc	0.0000897	Pa×s	721.67	Joback Method
dvisc	0.0001295	Pa×s	662.11	Joback Method
dvisc	0.0002012	Pa×s	602.55	Joback Method
dvisc	0.0003442	Pa×s	542.98	Joback Method
dvisc	0.0006723	Pa×s	483.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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