Isophthalic acid, 6-chlorohexyl heptyl ester

Inchi: InChI=1S/C21H31ClO4/c1-2-3-4-6-9-15-25-20(23)18-12-11-13-19(17-18)21(24)26-16-10
InchiKey: DHRBOFIVNIKSBM-UHFFFAOYSA-N
Formula: C21H31ClO4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCl)c1
Mol. weight [g/mol]: 382.92

Physical Properties

Property code	Value	Unit	Source
gf	-251.05	kJ/mol	Joback Method
hf	-757.05	kJ/mol	Joback Method
hfus	53.57	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.770		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2944.00		NIST Webbook
rinpol	2944.00		NIST Webbook
tb	901.55	K	Joback Method
tc	1108.65	K	Joback Method
tf	539.61	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.34	J/mol×K	901.55	Joback Method
cpg	979.52	J/mol×K	936.07	Joback Method
cpg	993.50	J/mol×K	970.58	Joback Method
cpg	1006.30	J/mol×K	1005.10	Joback Method
cpg	1017.96	J/mol×K	1039.62	Joback Method
cpg	1028.51	J/mol×K	1074.14	Joback Method
cpg	1037.97	J/mol×K	1108.65	Joback Method
dvisc	0.0004342	Pa×s	539.61	Joback Method

dvisc	0.0002402	Pa×s	599.93	Joback Method
dvisc	0.0001480	Pa×s	660.26	Joback Method
dvisc	0.0000989	Pa×s	720.58	Joback Method
dvisc	0.0000704	Pa×s	780.90	Joback Method
dvisc	0.0000526	Pa×s	841.23	Joback Method
dvisc	0.0000408	Pa×s	901.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345883&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

Latest version available from:
https://www.chemeo.com/cid/94-347-3/Isophthalic-acid-6-chlorohexyl-heptyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:02:44.859628512 +0000 UTC m=+3283027.496597760.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.