Terephthalic acid, 4-chloro-2-methylbenzyl heptyl ester

Inchi: InChI=1S/C23H27ClO4/c1-3-4-5-6-7-14-27-22(25)18-8-10-19(11-9-18)23(26)28-16-20-12

InchiKey: JIHGISJHPCNBCU-UHFFFAOYSA-N

Formula: C23H27ClO4

SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OCc2ccc(Cl)cc2C)cc1

Mol. weight [g/mol]: 402.91

Physical Properties

Property code	Value	Unit	Source
gf	-141.06	kJ/mol	Joback Method
hf	-584.74	kJ/mol	Joback Method
hfus	52.01	kJ/mol	Joback Method
hvap	96.03	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.133		Crippen Method
mcvol	314.530	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	3281.00		NIST Webbook
tb	983.95	K	Joback Method
tc	1212.54	K	Joback Method
tf	613.61	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.51	J/mol×K	983.95	Joback Method
cpg	990.27	J/mol×K	1022.05	Joback Method
cpg	1001.64	J/mol×K	1060.15	Joback Method
cpg	1011.65	J/mol×K	1098.25	Joback Method
cpg	1020.34	J/mol×K	1136.34	Joback Method
cpg	1027.76	J/mol×K	1174.44	Joback Method
cpg	1033.93	J/mol×K	1212.54	Joback Method
dvisc	0.0002483	Pa×s	613.61	Joback Method
dvisc	0.0001519	Pa×s	675.33	Joback Method

dvisc	0.0001009	Pa×s	737.06	Joback Method
dvisc	0.0000714	Pa×s	798.78	Joback Method
dvisc	0.0000531	Pa×s	860.50	Joback Method
dvisc	0.0000411	Pa×s	922.23	Joback Method
dvisc	0.0000329	Pa×s	983.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416112&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