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

Inchi: InChI=1S/C20H21ClO4/c1-3-4-11-24-19(22)15-5-7-16(8-6-15)20(23)25-13-17-9-10-18(21

InchiKey: LESRCXXYAGXCSW-UHFFFAOYSA-N

Formula: C20H21ClO4

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

Mol. weight [g/mol]: 360.83

Physical Properties

Property code	Value	Unit	Source
gf	-166.32	kJ/mol	Joback Method
hf	-522.82	kJ/mol	Joback Method
hfus	44.24	kJ/mol	Joback Method
hvap	89.35	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	4.962		Crippen Method
mcvol	272.260	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	915.31	K	Joback Method
tc	1144.16	K	Joback Method
tf	579.80	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.07	J/mol×K	915.31	Joback Method
cpg	814.66	J/mol×K	953.45	Joback Method
cpg	825.96	J/mol×K	991.59	Joback Method
cpg	836.00	J/mol×K	1029.74	Joback Method
cpg	844.79	J/mol×K	1067.88	Joback Method
cpg	852.38	J/mol×K	1106.02	Joback Method
cpg	858.78	J/mol×K	1144.16	Joback Method
dvisc	0.0003394	Pa×s	579.80	Joback Method

dvisc	0.0002149	Pa×s	635.72	Joback Method
dvisc	0.0001464	Pa×s	691.64	Joback Method
dvisc	0.0001057	Pa×s	747.56	Joback Method
dvisc	0.0000798	Pa×s	803.47	Joback Method
dvisc	0.0000625	Pa×s	859.39	Joback Method
dvisc	0.0000505	Pa×s	915.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416109&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