Terephthalic acid, butyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C20H30O4/c1-6-7-12-23-18(21)16-8-10-17(11-9-16)19(22)24-14-15(2)13-20(3

InchiKey: KAEOUMSRNWYSEN-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: CCCCOC(=O)c1ccc(C(=O)OCC(C)CC(C)(C)C)cc1

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-247.14	kJ/mol	Joback Method
hf	-734.70	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	79.68	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.873		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	837.57	K	Joback Method
tc	1044.90	K	Joback Method
tf	485.84	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.27	J/mol×K	837.57	Joback Method
cpg	895.72	J/mol×K	872.13	Joback Method
cpg	910.98	J/mol×K	906.68	Joback Method
cpg	925.11	J/mol×K	941.24	Joback Method
cpg	938.13	J/mol×K	975.79	Joback Method
cpg	950.10	J/mol×K	1010.35	Joback Method
cpg	961.05	J/mol×K	1044.90	Joback Method
dvisc	0.0006273	Pa×s	485.84	Joback Method

dvisc	0.0003093	Pa×s	544.46	Joback Method
dvisc	0.0001750	Pa×s	603.08	Joback Method
dvisc	0.0001095	Pa×s	661.70	Joback Method
dvisc	0.0000740	Pa×s	720.33	Joback Method
dvisc	0.0000530	Pa×s	778.95	Joback Method
dvisc	0.0000398	Pa×s	837.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416010&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