Terephthalic acid, 2-bromophenethyl isobutyl ester

Inchi: InChI=1S/C20H21BrO4/c1-14(2)13-25-20(23)17-9-7-16(8-10-17)19(22)24-12-11-15-5-3-4

InchiKey: XASREWGGLGBGTN-UHFFFAOYSA-N

Formula: C20H21BrO4

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCCc2ccccc2Br)cc1

Mol. weight [g/mol]: 405.28

Physical Properties

Property code	Value	Unit	Source
gf	-132.88	kJ/mol	Joback Method
hf	-474.56	kJ/mol	Joback Method
hfus	42.20	kJ/mol	Joback Method
hvap	90.35	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.661		Crippen Method
mcvol	277.520	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	938.62	K	Joback Method
tc	1175.56	K	Joback Method
tf	582.16	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.22	J/mol×K	938.62	Joback Method
cpg	826.45	J/mol×K	978.11	Joback Method
cpg	837.38	J/mol×K	1017.60	Joback Method
cpg	847.07	J/mol×K	1057.09	Joback Method
cpg	855.56	J/mol×K	1096.58	Joback Method
cpg	862.91	J/mol×K	1136.07	Joback Method
cpg	869.16	J/mol×K	1175.56	Joback Method
dvisc	0.0003364	Pa×s	582.16	Joback Method

dvisc	0.0002017	Pa×s	641.57	Joback Method
dvisc	0.0001318	Pa×s	700.98	Joback Method
dvisc	0.0000921	Pa×s	760.39	Joback Method
dvisc	0.0000678	Pa×s	819.80	Joback Method
dvisc	0.0000520	Pa×s	879.21	Joback Method
dvisc	0.0000412	Pa×s	938.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416023&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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