

Phthalic acid, butyl 2-trifluoromethylbenzyl ester

Other names:	Phthalic acid, butyl 2-trifluorobenzyl ester
Inchi:	InChI=1S/C20H19F3O4/c1-2-3-12-26-18(24)15-9-5-6-10-16(15)19(25)27-13-14-8-4-7-11
InchiKey:	RLNMEGLWDAXFFJ-UHFFFAOYSA-N
Formula:	C20H19F3O4
SMILES:	CCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]:	380.36

Physical Properties

Property code	Value	Unit	Source
gf	-726.35	kJ/mol	Joback Method
hf	-1092.69	kJ/mol	Joback Method
hfus	42.26	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.019		Crippen Method
mcvol	265.330	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	2309.00		NIST Webbook
tb	867.48	K	Joback Method
tc	1081.23	K	Joback Method
tf	541.55	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.43	J/molxK	867.48	Joback Method
cpg	816.29	J/molxK	903.10	Joback Method
cpg	828.02	J/molxK	938.73	Joback Method
cpg	838.69	J/molxK	974.35	Joback Method
cpg	848.34	J/molxK	1009.98	Joback Method
cpg	857.02	J/molxK	1045.60	Joback Method
cpg	864.78	J/molxK	1081.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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