

Terephthalic acid, di(2,5-difluorobenzyl) ester

Inchi: InChI=1S/C22H14F4O4/c23-17-5-7-19(25)15(9-17)11-29-21(27)13-1-2-14(4-3-13)22(28)
InchiKey: KOEHVNBWMNTUOF-UHFFFAOYSA-N
Formula: C22H14F4O4
SMILES: O=C(OCc1cc(F)ccc1F)c1ccc(C(=O)OCc2cc(F)ccc2F)cc1
Mol. weight [g/mol]: 418.34

Physical Properties

Property code	Value	Unit	Source
gf	-823.64	kJ/mol	Joback Method
hf	-1119.21	kJ/mol	Joback Method
hfus	50.81	kJ/mol	Joback Method
hvap	89.75	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	4.957		Crippen Method
mvol	271.520	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
tb	957.36	K	Joback Method
tc	1184.98	K	Joback Method
tf	626.24	K	Joback Method
vc	1.063	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.77	J/molxK	957.36	Joback Method
cpg	825.73	J/molxK	995.30	Joback Method
cpg	834.40	J/molxK	1033.23	Joback Method
cpg	841.81	J/molxK	1071.17	Joback Method
cpg	848.01	J/molxK	1109.11	Joback Method
cpg	853.01	J/molxK	1147.04	Joback Method
cpg	856.85	J/molxK	1184.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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