2,4-DB, PFB

Other names: 2,4-DB, PFB ester
Inchi: InChI=1S/C17H11Cl2F5O3/c18-8-3-4-11(10(19)6-8)26-5-1-2-12(25)27-7-9-13(20)15(22)
InchiKey: PNIWBAIIZMIMHJ-UHFFFAOYSA-N
Formula: C17H11Cl2F5O3
SMILES: O=C(CCCOc1ccc(Cl)cc1Cl)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 429.17

Physical Properties

Property code	Value	Unit	Source
gf	-1087.16	kJ/mol	Joback Method
hf	-1390.49	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.591		Crippen Method
mcvol	249.510	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2319.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	846.50	K	Joback Method
tc	1050.67	K	Joback Method
tf	579.01	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.72	J/mol×K	846.50	Joback Method
cpg	687.00	J/mol×K	880.53	Joback Method
cpg	696.38	J/mol×K	914.56	Joback Method
cpg	704.86	J/mol×K	948.59	Joback Method

cpg	712.43	J/mol×K	982.61	Joback Method
cpg	719.10	J/mol×K	1016.64	Joback Method
cpg	724.87	J/mol×K	1050.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13955&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

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
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