

Succinic acid, di(2-(pentafluorophenoxy)ethyl) ester

Inchi: InChI=1S/C20H12F10O6/c21-9-11(23)15(27)19(16(28)12(9)24)35-5-3-33-7(31)1-2-8(32)

InchiKey: XVNYKLBSUBGLLU-UHFFFAOYSA-N

Formula: C20H12F10O6

SMILES: O=C(CCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F)OCCOc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 538.29

Physical Properties

Property code	Value	Unit	Source
gf	-2379.90	kJ/mol	Joback Method
hf	-2812.91	kJ/mol	Joback Method
hfus	70.50	kJ/mol	Joback Method
hvap	86.25	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	4.402		Crippen Method
mvol	289.460	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	950.28	K	Joback Method
tc	1168.01	K	Joback Method
tf	687.88	K	Joback Method
vc	1.204	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.79	J/mol×K	950.28	Joback Method
cpg	903.30	J/mol×K	986.57	Joback Method
cpg	911.27	J/mol×K	1022.86	Joback Method
cpg	917.64	J/mol×K	1059.14	Joback Method
cpg	922.36	J/mol×K	1095.43	Joback Method
cpg	925.40	J/mol×K	1131.72	Joback Method
cpg	926.71	J/mol×K	1168.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381559&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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