

Diethylmalonic acid, octyl pentafluorophenyl ester

Inchi:	InChI=1S/C21H27F5O4/c1-4-7-8-9-10-11-12-29-19(27)21(5-2,6-3)20(28)30-18-16(25)14
InchiKey:	BCUDDIXAHXMQKA-UHFFFAOYSA-N
Formula:	C21H27F5O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	438.43

Physical Properties

Property code	Value	Unit	Source
gf	-1248.85	kJ/mol	Joback Method
hf	-1776.49	kJ/mol	Joback Method
hfus	55.80	kJ/mol	Joback Method
hvap	80.86	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	5.998		Crippen Method
mcvol	306.720	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpola	2090.00		NIST Webbook
rinpola	2090.00		NIST Webbook
tb	877.16	K	Joback Method
tc	1074.10	K	Joback Method
tf	565.14	K	Joback Method
vc	1.230	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.43	J/molxK	877.16	Joback Method
cpg	986.11	J/molxK	909.98	Joback Method
cpg	999.70	J/molxK	942.81	Joback Method
cpg	1012.24	J/molxK	975.63	Joback Method
cpg	1023.73	J/molxK	1008.45	Joback Method
cpg	1034.21	J/molxK	1041.27	Joback Method
cpg	1043.70	J/molxK	1074.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370215&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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