

Glutaric acid, heptyl 2-(pentafluorophenoxy)ethyl ester

Inchi:	InChI=1S/C20H25F5O5/c1-2-3-4-5-6-10-28-13(26)8-7-9-14(27)29-11-12-30-20-18(24)16
InchiKey:	CMNQTCRTJVGEJG-UHFFFAOYSA-N
Formula:	C20H25F5O5
SMILES:	CCCCCCCOC(=O)CCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	440.40

Physical Properties

Property code	Value	Unit	Source
gf	-1365.11	kJ/mol	Joback Method
hf	-1879.32	kJ/mol	Joback Method
hfus	61.81	kJ/mol	Joback Method
hvap	82.34	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	4.988		Crippen Method
mvol	298.500	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	879.93	K	Joback Method
tc	1077.35	K	Joback Method
tf	573.68	K	Joback Method
vc	1.204	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.32	J/molxK	879.93	Joback Method
cpg	954.49	J/molxK	912.83	Joback Method
cpg	967.48	J/molxK	945.74	Joback Method
cpg	979.28	J/molxK	978.64	Joback Method
cpg	989.90	J/molxK	1011.54	Joback Method
cpg	999.32	J/molxK	1044.45	Joback Method
cpg	1007.53	J/molxK	1077.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377327&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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