

Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H11Cl3F8O4/c17-7-4-9(19)10(5-8(7)18)31-12(29)3-1-2-11(28)30-6-14(22,23)15

InchiKey: VUCXUOHDJKRMSY-UHFFFAOYSA-N

Formula: C16H11Cl3F8O4

SMILES: O=C(CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 525.60

Physical Properties

Property code	Value	Unit	Source
gf	-1888.67	kJ/mol	Joback Method
hf	-2308.68	kJ/mol	Joback Method
hfus	47.11	kJ/mol	Joback Method
hvap	76.13	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.437		Crippen Method
mvol	278.300	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rmpol	2304.00		NIST Webbook
rmpol	2304.00		NIST Webbook
tb	856.00	K	Joback Method
tc	1053.76	K	Joback Method
tf	565.12	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.37	J/mol×K	856.00	Joback Method
cpg	793.40	J/mol×K	888.96	Joback Method
cpg	801.66	J/mol×K	921.92	Joback Method
cpg	809.21	J/mol×K	954.88	Joback Method
cpg	816.10	J/mol×K	987.84	Joback Method
cpg	822.41	J/mol×K	1020.80	Joback Method
cpg	828.19	J/mol×K	1053.76	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=U392155&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
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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