

# Glutaric acid, (2-chlorocyclohexyl)methyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

<b>Inchi:</b>	InChI=1S/C17H21ClF8O4/c18-11-5-2-1-4-10(11)8-29-12(27)6-3-7-13(28)30-9-15(21,22)
<b>InchiKey:</b>	SNMKZQDBSIBTRX-UHFFFAOYSA-N
<b>Formula:</b>	C17H21ClF8O4
<b>SMILES:</b>	O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)OCC1CCCCC1Cl
<b>Mol. weight [g/mol]:</b>	476.79

## Physical Properties

Property code	Value	Unit	Source
gf	-1923.17	kJ/mol	Joback Method
hf	-2465.98	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.212		Crippen Method
mvol	280.810	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	777.28	K	Joback Method
tc	958.79	K	Joback Method
tf	455.71	K	Joback Method
vc	1.121	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.75	J/molxK	777.28	Joback Method
cpg	901.52	J/molxK	807.53	Joback Method
cpg	915.23	J/molxK	837.78	Joback Method
cpg	927.94	J/molxK	868.03	Joback Method
cpg	939.70	J/molxK	898.28	Joback Method
cpg	950.55	J/molxK	928.54	Joback Method
cpg	960.56	J/molxK	958.79	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405440&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405440&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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