Glutaric acid, (2-chlorocyclohexyl)methyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C15H21ClF4O4/c16-11-5-2-1-4-10(11)8-23-12(21)6-3-7-13(22)24-9-15(19,20)1

InchiKey: NTHKUDADTQZNFB-UHFFFAOYSA-N

Formula: C15H21ClF4O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCC1CCCCC1Cl

Mol. weight [g/mol]: 376.77

Physical Properties

Property code	Value	Unit	Source
gf	-1166.45	kJ/mol	Joback Method
hf	-1622.76	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.941		Crippen Method
mcvol	245.550	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2026.00		NIST Webbook
rinpol	2026.00		NIST Webbook
tb	740.90	K	Joback Method
tc	928.09	K	Joback Method
tf	425.97	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.84	J/mol×K	740.90	Joback Method
cpg	754.46	J/mol×K	772.10	Joback Method
cpg	769.04	J/mol×K	803.30	Joback Method
cpg	782.60	J/mol×K	834.49	Joback Method
cpg	795.18	J/mol×K	865.69	Joback Method
cpg	806.78	J/mol×K	896.89	Joback Method
cpg	817.44	J/mol×K	928.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume