Glutaric acid, 2,2,3,3-tetrafluoropropyl 4-chlorobenzyl ester

Inchi: InChI=1S/C15H15ClF4O4/c16-11-6-4-10(5-7-11)8-23-12(21)2-1-3-13(22)24-9-15(19,20)1

InchiKey: OZKAQPKNVSYKCB-UHFFFAOYSA-N

Formula: C15H15ClF4O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 370.72

Physical Properties

Property code	Value	Unit	Source
gf	-1080.41	kJ/mol	Joback Method
hf	-1431.68	kJ/mol	Joback Method
hfus	39.41	kJ/mol	Joback Method
hvap	69.67	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.997		Crippen Method
mcvol	232.650	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	2043.00		NIST Webbook
rinpol	2043.00		NIST Webbook
tb	757.68	K	Joback Method
tc	950.09	K	Joback Method
tf	461.77	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.76	J/mol×K	757.68	Joback Method
cpg	665.87	J/mol×K	789.75	Joback Method
cpg	677.12	J/mol×K	821.82	Joback Method
cpg	687.53	J/mol×K	853.88	Joback Method
cpg	697.14	J/mol×K	885.95	Joback Method
cpg	705.98	J/mol×K	918.02	Joback Method
cpg	714.06	J/mol×K	950.09	Joback Method

Sources

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=U391721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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