Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C15H24F4O4/c1-4-6-11(10(2)3)23-13(21)8-5-7-12(20)22-9-15(18,19)14(16)17

InchiKey: RZZHVCKNFCUBLB-UHFFFAOYSA-N

Formula: C15H24F4O4

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

Mol. weight [g/mol]: 344.34

Physical Properties

Property code	Value	Unit	Source
gf	-1176.14	kJ/mol	Joback Method
hf	-1651.56	kJ/mol	Joback Method
hfus	34.52	kJ/mol	Joback Method
hvap	61.57	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.968		Crippen Method
mcvol	244.170	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
tb	687.71	K	Joback Method
tc	856.28	K	Joback Method
tf	362.91	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.43	J/mol×K	687.71	Joback Method
cpg	727.56	J/mol×K	715.80	Joback Method
cpg	741.90	J/mol×K	743.90	Joback Method
cpg	755.48	J/mol×K	771.99	Joback Method
cpg	768.31	J/mol×K	800.09	Joback Method
cpg	780.41	J/mol×K	828.18	Joback Method
cpg	791.80	J/mol×K	856.28	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=U393725&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