

Glutaric acid, hex-2-en-1-yl 2,2,3,3-tetrafluoropropyl ester

Inchi:	InChI=1S/C14H20F4O4/c1-2-3-4-5-9-21-11(19)7-6-8-12(20)22-10-14(17,18)13(15)16/h4
InchiKey:	YBHMFNOLXIDRW-SNAWJCMRSA-N
Formula:	C14H20F4O4
SMILES:	CCCC=CCOC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	328.30

Physical Properties

Property code	Value	Unit	Source
gf	-1099.46	kJ/mol	Joback Method
hf	-1503.14	kJ/mol	Joback Method
hfus	39.17	kJ/mol	Joback Method
hvap	60.08	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.500		Crippen Method
mvol	225.780	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	669.87	K	Joback Method
tc	838.32	K	Joback Method
tf	376.56	K	Joback Method
vc	0.902	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.98	J/mol×K	669.87	Joback Method
cpg	648.72	J/mol×K	697.94	Joback Method
cpg	661.75	J/mol×K	726.02	Joback Method
cpg	674.09	J/mol×K	754.09	Joback Method
cpg	685.77	J/mol×K	782.17	Joback Method
cpg	696.81	J/mol×K	810.24	Joback Method
cpg	707.23	J/mol×K	838.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405324&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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