

Glutaric acid, 2-norbornyl 2,2,3,3-tetrafluoropropyl ester

Inchi:	InChI=1S/C15H20F4O4/c16-14(17)15(18,19)8-22-12(20)2-1-3-13(21)23-11-7-9-4-5-10(1
InchiKey:	RIEJSVNXSMCSQD-UHFFFAOYSA-N
Formula:	C15H20F4O4
SMILES:	O=C(CCCC(=O)OC1CC2CCC1C2)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	340.31

Physical Properties

Property code	Value	Unit	Source
gf	-1069.57	kJ/mol	Joback Method
hf	-1521.90	kJ/mol	Joback Method
hfus	36.80	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.332		Crippen Method
mcvol	222.450	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	1793.00		NIST Webbook
rinpol	1793.00		NIST Webbook
tb	701.67	K	Joback Method
tc	884.45	K	Joback Method
tf	421.03	K	Joback Method
vc	0.883	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.18	J/mol×K	701.67	Joback Method
cpg	703.00	J/mol×K	732.13	Joback Method
cpg	717.86	J/mol×K	762.60	Joback Method
cpg	731.82	J/mol×K	793.06	Joback Method
cpg	744.93	J/mol×K	823.53	Joback Method
cpg	757.23	J/mol×K	853.99	Joback Method
cpg	768.77	J/mol×K	884.45	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U405483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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