

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

Inchi:	InChI=1S/C18H24F4O4/c1-17(2)12-7-6-11(13(17)8-12)9-25-14(23)4-3-5-15(24)26-10-18
InchiKey:	OTRQIIQYVQPCLY-UHFFFAOYSA-N
Formula:	C18H24F4O4
SMILES:	CC1(C)C2CC=C(COC(=O)CCCC(=O)OCC(F)(F)C(F)F)C1C2
Mol. weight [g/mol]:	380.37

Physical Properties

Property code	Value	Unit	Source
gf	-1029.47	kJ/mol	Joback Method
hf	-1522.27	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	68.51	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.136		Crippen Method
mvol	260.420	ml/mol	McGowan Method
pc	1382.99	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	774.69	K	Joback Method
tc	963.12	K	Joback Method
tf	492.02	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.15	J/molxK	774.69	Joback Method
cpg	842.51	J/molxK	806.10	Joback Method
cpg	858.26	J/molxK	837.50	Joback Method
cpg	873.51	J/molxK	868.91	Joback Method
cpg	888.37	J/molxK	900.31	Joback Method
cpg	902.95	J/molxK	931.72	Joback Method
cpg	917.35	J/molxK	963.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405536&Units=SI

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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