

Glutaric acid, 2,2,3,3-tetrafluoropropyl oct-3-en-2-yl ester

Inchi: InChI=1S/C16H24F4O4/c1-3-4-5-6-8-12(2)24-14(22)10-7-9-13(21)23-11-16(19,20)15(17)
InchiKey: NNGFFFMZNGODGX-SOFGYWHQSA-N
Formula: C16H24F4O4
SMILES: CCCCC=CC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 356.35

Physical Properties

Property code	Value	Unit	Source
gf	-1085.06	kJ/mol	Joback Method
hf	-1549.70	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.278		Crippen Method
mvol	253.960	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
tb	715.19	K	Joback Method
tc	887.05	K	Joback Method
tf	384.10	K	Joback Method
vc	1.008	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.66	J/mol×K	715.19	Joback Method
cpg	759.51	J/mol×K	743.83	Joback Method
cpg	773.57	J/mol×K	772.48	Joback Method
cpg	786.85	J/mol×K	801.12	Joback Method
cpg	799.39	J/mol×K	829.76	Joback Method
cpg	811.21	J/mol×K	858.40	Joback Method
cpg	822.35	J/mol×K	887.05	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=U393982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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