

Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-fluoroethyl ester

Inchi:	InChI=1S/C12H13F9O4/c13-4-5-24-7(22)2-1-3-8(23)25-6-10(16,17)12(20,21)11(18,19)9
InchiKey:	SBLUZSKHWBSZSZ-UHFFFAOYSA-N
Formula:	C12H13F9O4
SMILES:	O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)OCCF
Mol. weight [g/mol]:	392.21

Physical Properties

Property code	Value	Unit	Source
gf	-2164.89	kJ/mol	Joback Method
hf	-2577.13	kJ/mol	Joback Method
hfus	34.37	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.384		Crippen Method
mcvol	210.750	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinqol	1436.00		NIST Webbook
tb	609.84	K	Joback Method
tc	760.73	K	Joback Method
tf	366.89	K	Joback Method
vc	0.878	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.14	J/molxK	609.84	Joback Method
cpg	610.08	J/molxK	634.99	Joback Method
cpg	621.36	J/molxK	660.14	Joback Method
cpg	632.00	J/molxK	685.28	Joback Method
cpg	642.04	J/molxK	710.43	Joback Method
cpg	651.49	J/molxK	735.58	Joback Method
cpg	660.38	J/molxK	760.73	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=U393704&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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