

Glutaric acid, 2,2,3,3-tetrafluoropropyl 3-methyl-5-methoxypentyl ester

Inchi:	InChI=1S/C15H24F4O5/c1-11(6-8-22-2)7-9-23-12(20)4-3-5-13(21)24-10-15(18,19)14(16)
InchiKey:	UKFQVTOIZBWMIX-UHFFFAOYSA-N
Formula:	C15H24F4O5
SMILES:	COCCC(C)CCOC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	360.34

Physical Properties

Property code	Value	Unit	Source
gf	-1278.70	kJ/mol	Joback Method
hf	-1778.50	kJ/mol	Joback Method
hfus	39.23	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.206		Crippen Method
mcvol	250.040	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
tb	710.57	K	Joback Method
tc	879.21	K	Joback Method
tf	400.14	K	Joback Method
vc	0.991	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.05	J/mol×K	710.57	Joback Method
cpg	755.84	J/mol×K	738.68	Joback Method
cpg	769.86	J/mol×K	766.78	Joback Method
cpg	783.12	J/mol×K	794.89	Joback Method
cpg	795.61	J/mol×K	822.99	Joback Method
cpg	807.36	J/mol×K	851.10	Joback Method
cpg	818.37	J/mol×K	879.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393515&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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