

Glutaric acid, 2,2,2-trifluoroethyl nonyl ester

Inchi: InChI=1S/C16H27F3O4/c1-2-3-4-5-6-7-8-12-22-14(20)10-9-11-15(21)23-13-16(17,18)19
InchiKey: AAQTYANFWTTWPP-UHFFFAOYSA-N
Formula: C16H27F3O4
SMILES: CCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 340.38

Physical Properties

Property code	Value	Unit	Source
gf	-965.59	kJ/mol	Joback Method
hf	-1460.25	kJ/mol	Joback Method
hfus	44.60	kJ/mol	Joback Method
hvap	65.78	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.556		Crippen Method
mcvol	256.490	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	1821.00		NIST Webbook
rinpol	1821.00		NIST Webbook
tb	712.64	K	Joback Method
tc	881.61	K	Joback Method
tf	418.59	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.99	J/molxK	712.64	Joback Method
cpg	774.48	J/molxK	740.80	Joback Method
cpg	789.19	J/molxK	768.96	Joback Method
cpg	803.12	J/molxK	797.12	Joback Method
cpg	816.31	J/molxK	825.28	Joback Method
cpg	828.76	J/molxK	853.45	Joback Method
cpg	840.50	J/molxK	881.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380516&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
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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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