

Glutaric acid, 2-(cyclohexyl)ethyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H24F4O4/c17-15(18)16(19,20)11-24-14(22)8-4-7-13(21)23-10-9-12-5-2-1-
InchiKey: FRAUWDORAJPUNM-UHFFFAOYSA-N
Formula: C16H24F4O4
SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCCC1CCCCC1
Mol. weight [g/mol]: 356.35

Physical Properties

Property code	Value	Unit	Source
gf	-1138.39	kJ/mol	Joback Method
hf	-1607.32	kJ/mol	Joback Method
hfus	35.99	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.114		Crippen Method
mvol	247.400	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	1867.00		NIST Webbook
rinpol	1867.00		NIST Webbook
tb	731.02	K	Joback Method
tc	913.82	K	Joback Method
tf	411.56	K	Joback Method
vc	0.968	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.16	J/molxK	731.02	Joback Method
cpg	778.76	J/molxK	761.49	Joback Method
cpg	794.33	J/molxK	791.95	Joback Method
cpg	808.90	J/molxK	822.42	Joback Method
cpg	822.49	J/molxK	852.89	Joback Method
cpg	835.12	J/molxK	883.36	Joback Method
cpg	846.84	J/molxK	913.82	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=U405412&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
hvap:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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