Glutaric acid, (2-methylcyclohex-1-enyl)methyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C16H23F3O4/c1-11-6-3-4-7-13(11)10-22-14(20)8-5-9-15(21)23-12(2)16(17,18)
InchiKey: XJSGKRQDRAFMQI-UHFFFAOYSA-N
Formula: C16H23F3O4
SMILES: CC1=C(COC(=O)CCCC(=O)OC(C)C(F)(F)F)CCCC1
Mol. weight [g/mol]: 336.35

Physical Properties

Property code	Value	Unit	Source
gf	-925.17	kJ/mol	Joback Method
hf	-1356.03	kJ/mol	Joback Method
hfus	32.28	kJ/mol	Joback Method
hvap	67.74	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.084		Crippen Method
mcvol	241.330	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1783.00		NIST Webbook
tb	745.54	K	Joback Method
tc	936.56	K	Joback Method
tf	441.01	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.46	J/mol×K	745.54	Joback Method
cpg	741.11	J/mol×K	777.38	Joback Method
cpg	755.77	J/mol×K	809.21	Joback Method
cpg	769.45	J/mol×K	841.05	Joback Method
cpg	782.18	J/mol×K	872.89	Joback Method
cpg	793.99	J/mol×K	904.72	Joback Method
cpg	804.91	J/mol×K	936.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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