Glutaric acid, di(3-methylbut-2-enyl) ester

Inchi: InChI=1S/C15H24O4/c1-12(2)8-10-18-14(16)6-5-7-15(17)19-11-9-13(3)4/h8-9H,5-7,10-1
InchiKey: JLCZUSIQPYBWPA-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: CC(C)=CCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-249.08	kJ/mol	Joback Method
hf	-627.67	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	67.37	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.175		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	1926.00		NIST Webbook
tb	703.26	K	Joback Method
tc	893.66	K	Joback Method
tf	365.05	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.14	J/mol×K	703.26	Joback Method
cpg	646.58	J/mol×K	734.99	Joback Method
cpg	661.21	J/mol×K	766.73	Joback Method
cpg	675.06	J/mol×K	798.46	Joback Method
cpg	688.16	J/mol×K	830.19	Joback Method
cpg	700.53	J/mol×K	861.92	Joback Method
cpg	712.19	J/mol×K	893.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360097&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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