

Glutaric acid, but-3-en-2-yl 8-chlorooctyl ester

Inchi:	InChI=1S/C17H29ClO4/c1-3-15(2)22-17(20)12-10-11-16(19)21-14-9-7-5-4-6-8-13-18/h3,
InchiKey:	YQLZRXWPQLLFFA-UHFFFAOYSA-N
Formula:	C17H29ClO4
SMILES:	<chem>C=CC(C)OC(=O)CCCC(=O)OCCCCCCCCCI</chem>
Mol. weight [g/mol]:	332.86

Physical Properties

Property code	Value	Unit	Source
gf	-302.11	kJ/mol	Joback Method
hf	-779.40	kJ/mol	Joback Method
hfus	44.75	kJ/mol	Joback Method
hvap	75.08	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.397		Crippen Method
mvol	273.210	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2265.00		NIST Webbook
rinpol	2265.00		NIST Webbook
tb	774.61	K	Joback Method
tc	960.05	K	Joback Method
tf	438.83	K	Joback Method
vc	1.060	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.02	J/molxK	774.61	Joback Method
cpg	812.76	J/molxK	805.52	Joback Method
cpg	827.59	J/molxK	836.42	Joback Method
cpg	841.54	J/molxK	867.33	Joback Method
cpg	854.61	J/molxK	898.23	Joback Method
cpg	866.83	J/molxK	929.14	Joback Method
cpg	878.21	J/molxK	960.05	Joback Method
dvisc	0.0010911	Paxs	438.83	Joback Method

dvisc	0.0005313	Paxs	494.79	Joback Method
dvisc	0.0002995	Paxs	550.76	Joback Method
dvisc	0.0001876	Paxs	606.72	Joback Method
dvisc	0.0001272	Paxs	662.68	Joback Method
dvisc	0.0000916	Paxs	718.65	Joback Method
dvisc	0.0000692	Paxs	774.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405245&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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