

Glutaric acid, 8-chlorooctyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C20H37ClO4/c1-4-12-18(17(2)3)25-20(23)14-11-13-19(22)24-16-10-8-6-5-7-9
InchiKey:	NXWWHZAUJRYBIB-UHFFFAOYSA-N
Formula:	C20H37ClO4
SMILES:	CCCC(OC(=O)CCCC(=O)OCCCCCCCCCI)C(C)C
Mol. weight [g/mol]:	376.96

Physical Properties

Property code	Value	Unit	Source
gf	-367.13	kJ/mol	Joback Method
hf	-972.03	kJ/mol	Joback Method
hfus	50.28	kJ/mol	Joback Method
hvap	82.03	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.647		Crippen Method
mcvol	319.780	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
tb	846.13	K	Joback Method
tc	1038.10	K	Joback Method
tf	459.40	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.79	J/molxK	846.13	Joback Method
cpg	1077.95	J/molxK	1006.10	Joback Method
cpg	1064.88	J/molxK	974.11	Joback Method
cpg	1050.75	J/molxK	942.11	Joback Method
cpg	1035.54	J/molxK	910.12	Joback Method
cpg	1019.23	J/molxK	878.12	Joback Method
cpg	1089.97	J/molxK	1038.10	Joback Method
dvisc	0.0000383	Paxs	846.13	Joback Method

dvisc	0.0000522	Paxs	781.67	Joback Method
dvisc	0.0000752	Paxs	717.22	Joback Method
dvisc	0.0001164	Paxs	652.76	Joback Method
dvisc	0.0001984	Paxs	588.31	Joback Method
dvisc	0.0003855	Paxs	523.86	Joback Method
dvisc	0.0009028	Paxs	459.40	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=U393843&Units=SI

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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