

Glutaric acid, 2,3-dichlorophenyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H24Cl2O4/c1-4-7-14(12(2)3)23-16(21)10-6-11-17(22)24-15-9-5-8-13(19)18
InchiKey:	SOEUJDUFZYMFCU-UHFFFAOYSA-N
Formula:	C18H24Cl2O4
SMILES:	CCCC(OC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl)C(C)C
Mol. weight [g/mol]:	375.29

Physical Properties

Property code	Value	Unit	Source
gf	-302.75	kJ/mol	Joback Method
hf	-732.90	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.437		Crippen Method
mvol	280.080	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	2478.00		NIST Webbook
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tb	874.44	K	Joback Method
tc	1088.12	K	Joback Method
tf	518.24	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.55	J/molxK	874.44	Joback Method
cpg	869.65	J/molxK	1052.50	Joback Method
cpg	860.66	J/molxK	1016.89	Joback Method
cpg	850.57	J/molxK	981.28	Joback Method
cpg	839.37	J/molxK	945.67	Joback Method
cpg	827.04	J/molxK	910.05	Joback Method
cpg	877.56	J/molxK	1088.12	Joback Method
dvisc	0.0000460	Paxs	874.44	Joback Method

dvisc	0.0000595	Paxs	815.07	Joback Method
dvisc	0.0000801	Paxs	755.71	Joback Method
dvisc	0.0001135	Paxs	696.34	Joback Method
dvisc	0.0001717	Paxs	636.97	Joback Method
dvisc	0.0002828	Paxs	577.61	Joback Method
dvisc	0.0005220	Paxs	518.24	Joback Method

Sources

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=U393825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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