

Fumaric acid, 8-chlorooctyl dodecyl ester

Inchi:	InChI=1S/C24H43ClO4/c1-2-3-4-5-6-7-8-10-13-16-21-28-23(26)18-19-24(27)29-22-17-14
InchiKey:	DKCGWVWEACHCBBJ-VHEBQXMUSA-N
Formula:	C24H43ClO4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	431.05

Physical Properties

Property code	Value	Unit	Source
gf	-248.35	kJ/mol	Joback Method
hf	-926.81	kJ/mol	Joback Method
hfus	67.89	kJ/mol	Joback Method
hvap	91.67	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.129		Crippen Method
mvol	371.840	ml/mol	McGowan Method
pc	857.47	kPa	Joback Method
rinpol	3125.00		NIST Webbook
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tb	942.69	K	Joback Method
tc	1156.01	K	Joback Method
tf	529.40	K	Joback Method
vc	1.456	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.74	J/molxK	942.69	Joback Method
cpg	1301.44	J/molxK	1120.46	Joback Method
cpg	1287.76	J/molxK	1084.91	Joback Method
cpg	1272.91	J/molxK	1049.35	Joback Method
cpg	1256.82	J/molxK	1013.80	Joback Method
cpg	1239.45	J/molxK	978.24	Joback Method
cpg	1313.99	J/molxK	1156.01	Joback Method
dvisc	0.0000216	Paxs	942.69	Joback Method

dvisc	0.0000289	Paxs	873.81	Joback Method
dvisc	0.0000405	Paxs	804.93	Joback Method
dvisc	0.0000605	Paxs	736.05	Joback Method
dvisc	0.0000982	Paxs	667.16	Joback Method
dvisc	0.0001783	Paxs	598.28	Joback Method
dvisc	0.0003780	Paxs	529.40	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=U348538&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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