

Fumaric acid, isoheptyl 2,3,5,6-tetrachlorophenyl ester

Inchi: InChI=1S/C16H16Cl4O4/c1-9(2)4-3-7-23-12(21)5-6-13(22)24-16-14(19)10(17)8-11(18)15
InchiKey: ISIZDRAVGGKUKL-AATRIKPKSA-N
Formula: C16H16Cl4O4
SMILES: CC(C)CCCOC(=O)C=CC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 414.11

Physical Properties

Property code	Value	Unit	Source
gf	-280.05	kJ/mol	Joback Method
hf	-623.54	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	91.56	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.741		Crippen Method
mcvol	272.080	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2646.00		NIST Webbook
rinpol	2646.00		NIST Webbook
tb	918.10	K	Joback Method
tc	1145.61	K	Joback Method
tf	590.50	K	Joback Method
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.78	J/molxK	918.10	Joback Method
cpg	721.80	J/molxK	956.02	Joback Method
cpg	730.82	J/molxK	993.94	Joback Method
cpg	738.87	J/molxK	1031.86	Joback Method
cpg	745.96	J/molxK	1069.77	Joback Method
cpg	752.12	J/molxK	1107.69	Joback Method
cpg	757.36	J/molxK	1145.61	Joback Method
dvisc	0.0002859	Paxs	590.50	Joback Method

dvisc	0.0001838	Paxs	645.10	Joback Method
dvisc	0.0001266	Paxs	699.70	Joback Method
dvisc	0.0000921	Paxs	754.30	Joback Method
dvisc	0.0000699	Paxs	808.90	Joback Method
dvisc	0.0000549	Paxs	863.50	Joback Method
dvisc	0.0000444	Paxs	918.10	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=U348251&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
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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